

# The use of H<sub>2</sub> technology

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NATIONAL INSTITUTE OF CHEMISTRY

# NATIONAL INSTITUTE OF CHEMISTRY, SLOVENIA



 poslitev za nedoločen čas permanent position <b>34%</b>	 <b>46%</b>	<b>374</b> zaposlenih employees	 <b>54%</b>
 poslitev za določen čas temporary position <b>66%</b>	<b>45%</b>	 iz Slovenije from Slovenia <b>86%</b>	<b>55%</b>
 iz drugih držav from other countries <b>14%</b>	<b>49%</b>	<b>14%</b>	<b>51%</b>
 doktorandov PhD students <b>117</b>	<b>45%</b>	<b>117</b>	<b>55%</b>
 raziskovalcev researchers <b>160</b>	<b>57%</b>	<b>160</b>	<b>43%</b>
 povprečna starost average age <b>38,0</b>	<b>38,0</b>	0-7 let/years: 74 7-12 let/years: 26 >12 let/years: 60	<b>36,9</b>
 povprečna starost average age <b>38,0</b>	<b>38,0</b>	<30 let/years: 31% 30-40 let/years: 37% 40-50 let/years: 15% 50-60 let/years: 12% >60 let/years: 5%	<b>36,9</b>

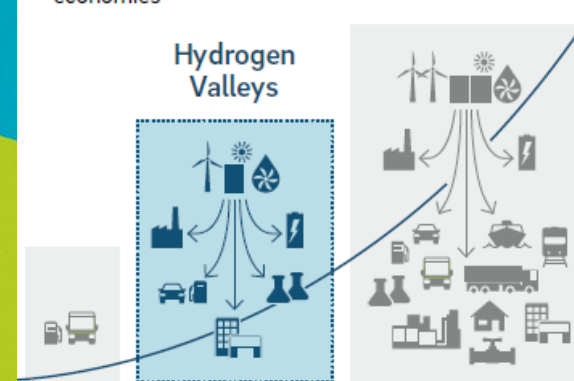


# Clean Hydrogen Partnership, Going Global, An update on Hydrogen Valleys and their role in the new hydrogen economy



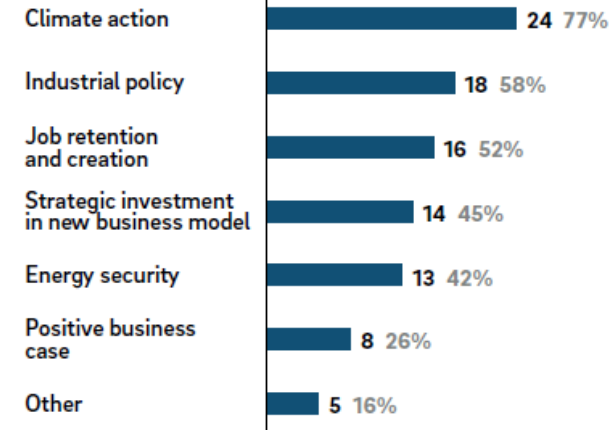
## THE AMBITION

- Next-generation market development
- Integrated (and larger-scale) projects covering more and more of the value chain – "mini hydrogen economies"



## THE UNDERLYING DRIVERS

Question: "What are the main drivers for your project?" (n=31)<sup>1</sup>



# H2GLASS – hydrogen/glass



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## DEMONSTRATION AND TRAINING CENTRE FOR CARBON-FREE TECHNOLOGIES

A bridge to accelerate the transfer of research knowledge to industry



### ABOUT THE INSTITUTE

The National Institute of Chemistry is a scientifically excellent, established and breakthrough **research institution** based in Slovenia, Europe, with 374 employees, of whom 167 have a PhD. The institute is a member of international multidisciplinary research networks and it collaborates with the best research institutions, groups and individuals worldwide.

### PILOT PLANTS FOR THE NEEDS OF INDUSTRY

The Centre will represent the link in the chain that will enable companies to increase the technological sophistication of their innovation in development. The Centre will include the development of all **green transition technologies**, such as hydrogen technologies, technologies for the capture and conversion of carbon dioxide, and especially the development of **modern battery technologies**.

### TRAINING

The Centre will facilitate the efficient transfer of knowledge, training employees in the companies the Centre cooperates with. The newly equipped Centre, enhanced with key personnel, will develop **programs for the transfer of knowledge and skills to the economy**, which, in addition to upgrading basic knowledge about advanced materials, will also enable practical training using **new high-tech equipment**.

### ESTABLISHMENT OF INFRASTRUCTURE THAT DOES NOT YET EXIST IN SLOVENIA

The Centre will enable both academic and industrial partners to confirm the concept of innovation in the field of developing advanced solutions for a **carbon-free society**, as well as enable the rapid transfer of innovation to higher levels of development, resulting in a faster market appearance.

### INTEGRATION INTO INTERNATIONAL FLOWS

The Centre will enable the involvement of researchers in the international research environment (with an emphasis on the European), put the National Institute of Chemistry and Slovenia on the map of scientifically **excellent organizations and countries**, and speed up the transfer of knowledge and experience into the international environment.

### EDUCATION

The Centre aims to fulfil the mission of transferring the knowledge and expertise of research work to younger generations of researchers and of students. In parallel with the increasing competencies in the international (European) research environment, the personnel will have access to the latest trends in research, which will significantly contribute to the expansion and enrichment of educational programs at the universities in Slovenia.

### CONNECTION WITH THE ECONOMY (SLOVENIAN AND FOREIGN)

The Centre will enable partner companies to access infrastructure that is otherwise inaccessible to them, or that would require a lot of investment funds that the companies do not have. The available infrastructure will also enable the easier networking of the Centre with industrial partners.

### THE MAIN ACTIVITIES OF THE CENTRE

- Validation of advanced materials
- Testing in industrial applications
- Standardization of the use of new materials and chemicals
- The development of business models for advanced technologies
- Quality assurance



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### GET IN TOUCH

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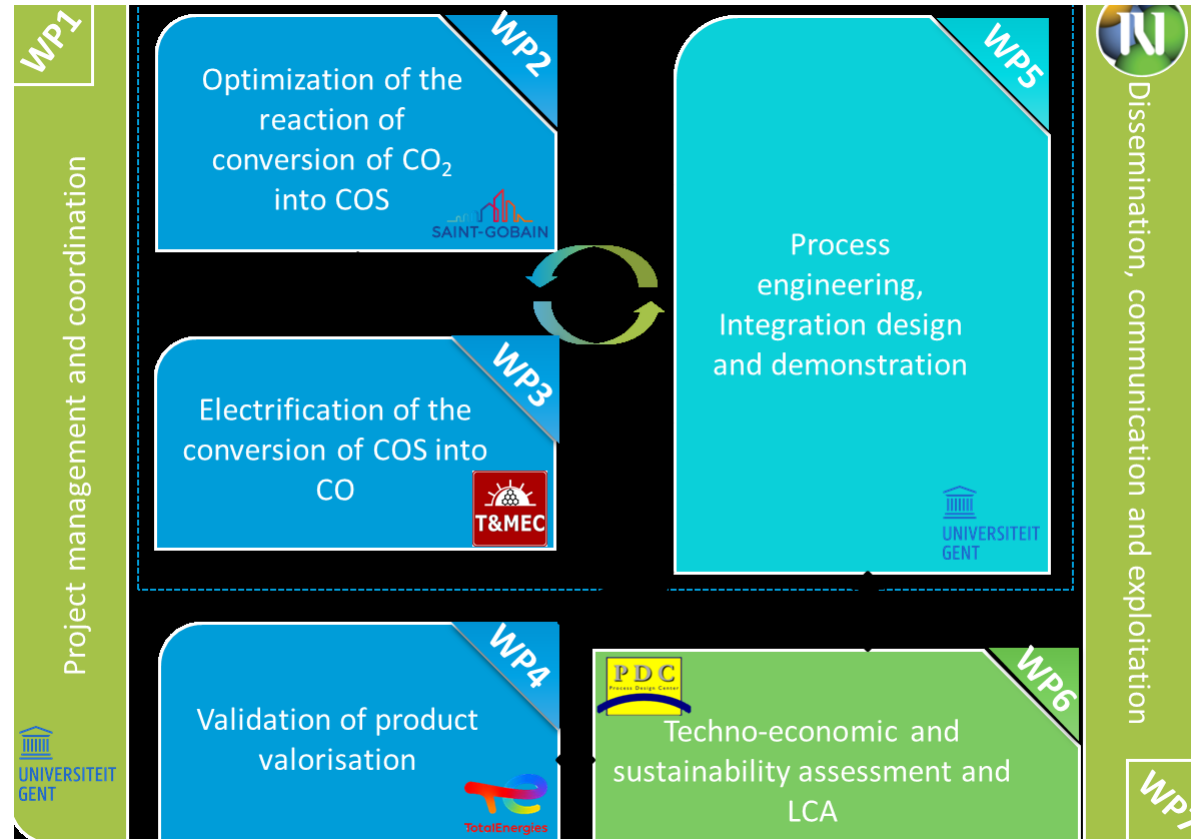




# HYPER – hydrogen/hydrogen peroxide

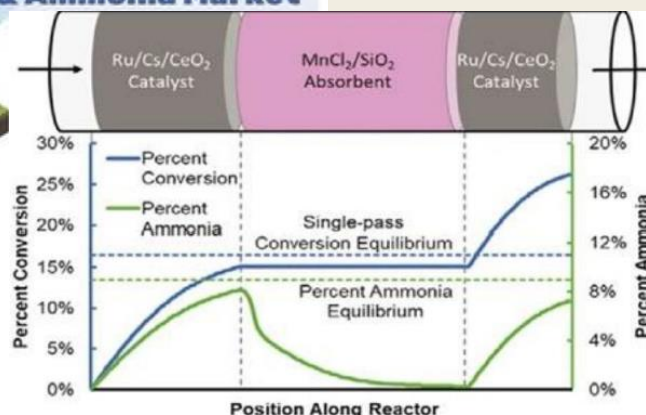


# E-CODUCT – hydrogen/sulphur



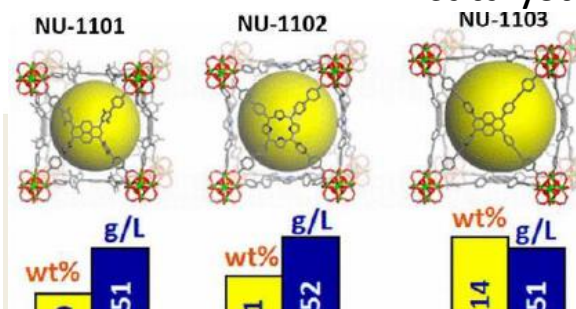
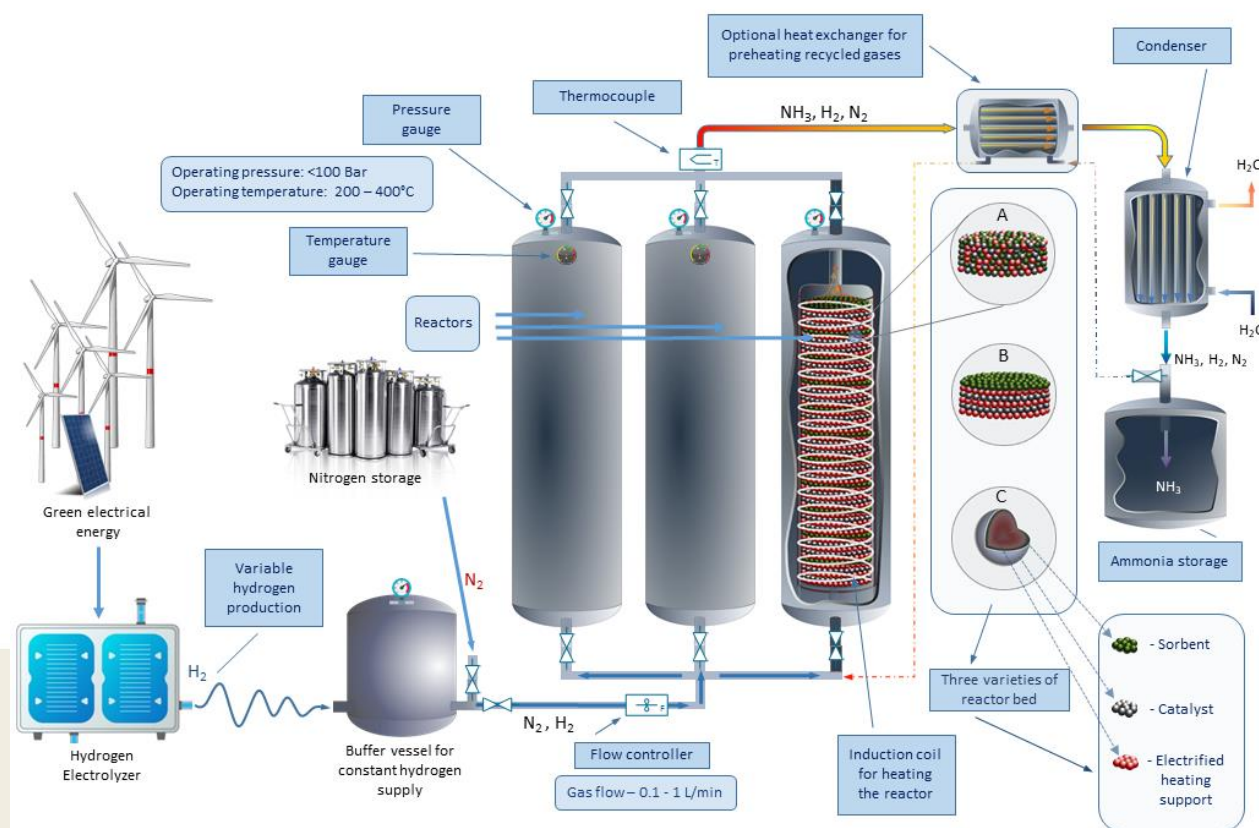


## Facilitating the European Hydrogen Economy & Ammonia Market



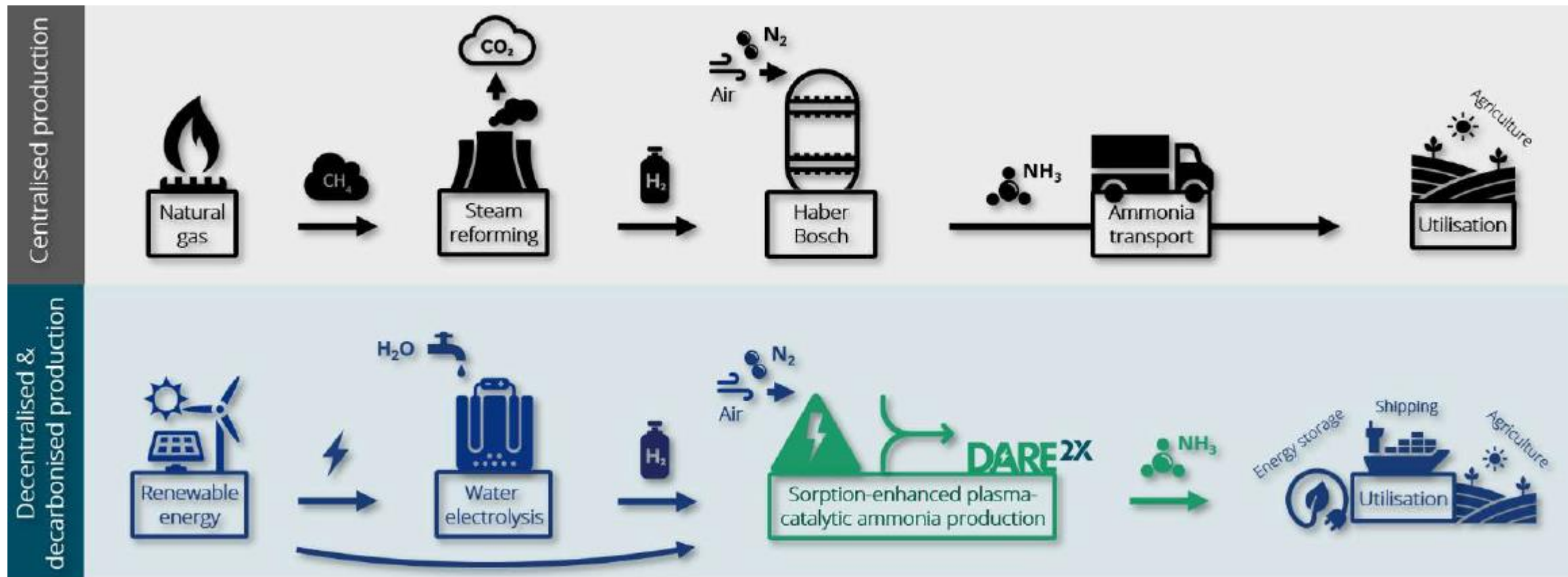
HySTrAm builds on developing physical H<sub>2</sub> storage materials, enabling short term storage (buffering renewables dynamics). The project will demonstrate a compact containerised ammonia synthesis system which is based on two main consecutive stages:

- 1) A short-term storage hydrogen vessel which will serve as a buffer to store and transport the hydrogen produced by electrolysis. Within the hydrogen vessel, new ultraporous material will be identified and optimised through machine learning technology
- 2) An ammonia synthesis reactor based on an improved the Haber-Bosch process where the stored hydrogen will react with nitrogen to form ammonia using the novel catalysts and sorbents developed in



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101022738.

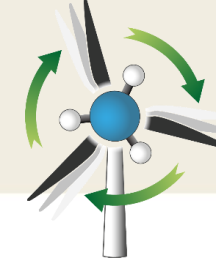






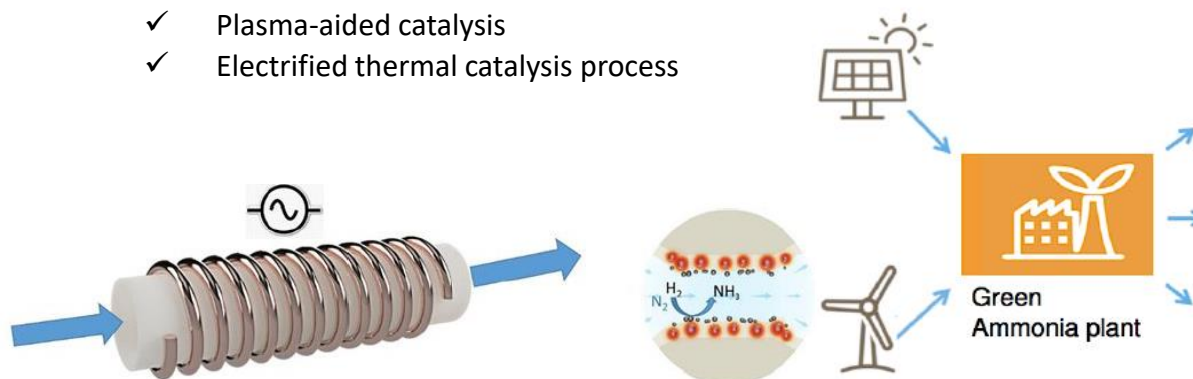
# Electrified ammonia production

Reduce impact of ammonia production processes on the environment



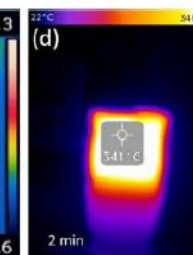
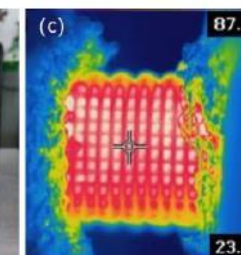
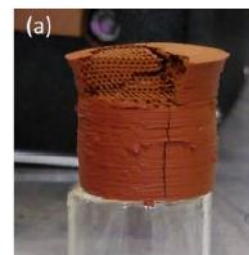
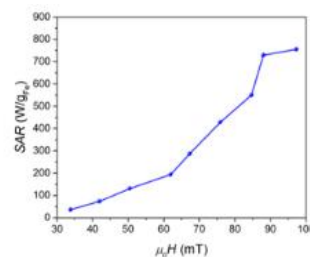
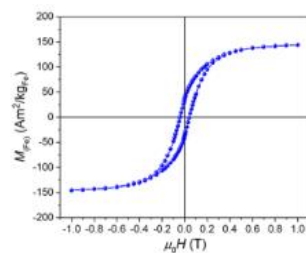
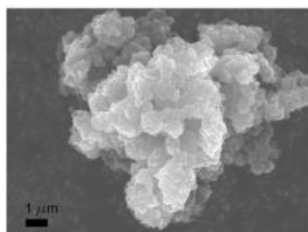
**ORACLE**  
三人寄れば文殊の知恵

- ✓ Novel routes and catalysts for synthesis of ammonia as alternative renewable fuel
  - ✓ Electrocatalysis
  - ✓ Plasma-aided catalysis
  - ✓ Electrified thermal catalysis process



## GREEN Market segments and applications

Green chemicals	1. High value chemicals (Specialty / pharma)	Developing segments
	2. Polymers and plastics / other	
Fertiliser	1. High value crops	Existing segments
	2. Other crops	
Energy <b>ORACLE</b>	1. Fuel (mobility/industry)	New segments
	2. Energy distribution	
	3. Storage / dispatchable power	



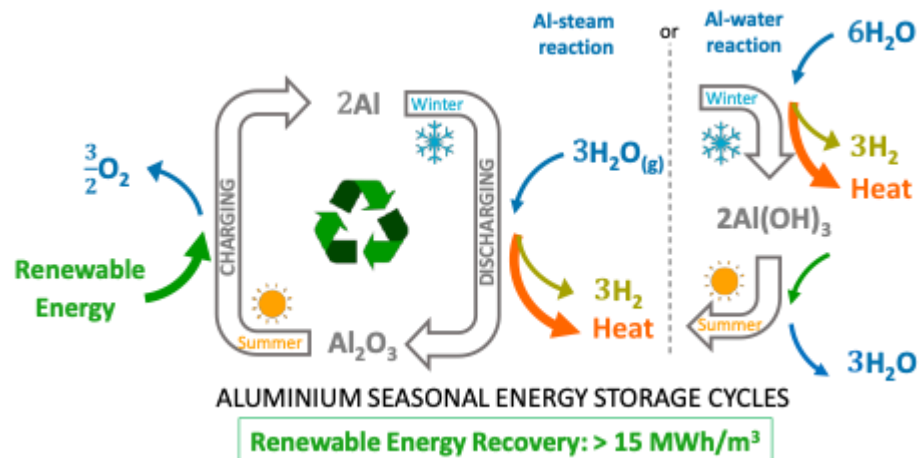
1. [Horizon 2020 project](#) - ORACLE, 2021-2024, 2.8 mil EUR
2. S. Gyergyek, M. Grilc, B. Likozar, D. Makovec. *Green chemistry*, 2022, 8
3. S. Gyergyek, D. Lisjak, M. Beković, M. Grilc, B. Likozar, M. Nečemer, D. Makovec. *Nanomaterials*, 2020, 10, 6, 1142.



## Going to very diverse sectors...

REVEAL project develops a game-changing and unique solution to this challenge, using the conversion of **aluminium oxide into aluminium metal** (Power-to-Al) in an environmentally friendly way to store renewable energy and produce a "renewable fuel" in the form of aluminium.

DINAMINE aims to demonstrate a holistic **mine management approach**, based on (i) artificial intelligence-based data analytics tools for real-time mine-to-port monitoring of the risks, performance, environmental footprint, maintenance needs, product quality and recovery rates, (ii) machine automation and robotization strategies to enhance safety and productivity, (iii) on-site studies to identify best practices for carbon neutral logistics/transportation, more energy-efficient processing, and waste/tailings handling and valorisation.





# PILOTS

## HYDROGEN (H<sub>2</sub>)



### About the Pilot

Hydrogen has become a bustling field of interest as more and more European nations voice their ambitions to unlock hydrogen as a sustainable source of energy that will contribute to the decarbonisation agenda in multiple ways. Hydrogen is expected to play an important role as an energy carrier in this decade. It enables efficient and affordable energy transmission over long distances, storage of surplus electricity and environmentally friendly mobility, especially over long distances.

In July 2020, the European Commission published their 'Hydrogen Strategy for a Climate-Neutral Europe' in line with the European Green Deal, which is setting a strategic objective to install at least 40GW of renewable hydrogen electrolyzers by 2030 and to produce up to 10 million tonnes of renewable hydrogen in the EU.

Recent developments in the energy sector have also propelled interest in clean, locally produced energy. Regions are at the forefront of the development of a hydrogen economy in Europe. How much clean hydrogen a region



#### CO-LEADING REGIONS

 Lombardia Małopolska Slovenia



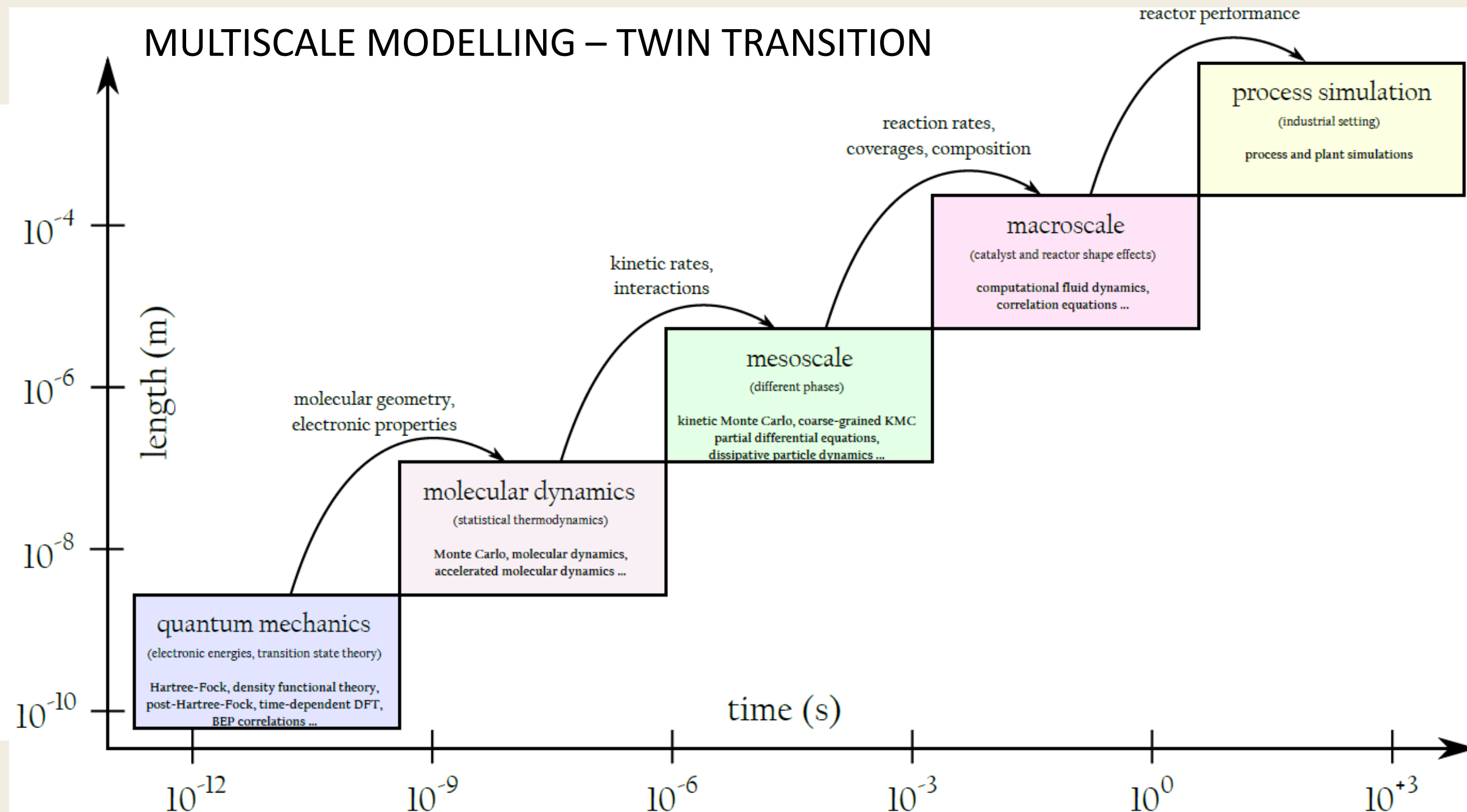
## Hydrogen? Yes, but not necessarily always.

### **The BEAR Project: HyBrid REgenerative glAss fuRnace (Innovation Fund 2022)**

- The BEAR project aims to decarbonise the end fired regenerative furnace design, which is the current state of the art in EU's production of packaging glass, by combining it with the more energy-efficient all-electric furnace concept into a hybrid regenerative furnace.
- The project will demonstrate a first-of-a-kind hybrid end-fired regenerative furnace with a more than 40% electrical melting share and an output capacity of 170 tons of glass per day. The furnace will be implemented in Steklarna Hrastnik's existing production site in Hrastnik, Zasavje, a Slovenian coal region in transition. The furnace will replace the existing end-fired regenerative furnace for extra-white flint glass production, resulting in a more than 50% reduction of natural gas consumption and up to 35% of greenhouse gas emissions savings.
- This hybrid furnace makes it possible to use a high share of carbon-neutral energy sources, while maintaining the operational flexibility of conventional regenerative furnaces, both in terms of output flexibility as well as cullet rate.
- This project will help align the glass melting process with the availability of renewable energy and open up glass manufacturing to provide ancillary services. The BEAR project will help avoid 96 384 tonnes CO<sub>2</sub>eq in its first 10 years of operation.



# MULTISCALE MODELLING – TWIN TRANSITION



# COMPUTATIONAL EQUIPMENT

**We have computational power on three scales (depending on the size of the problem)**

## **1. Working stations**

Typical 8-cores PCs with 32 GB RAM and RTX3080 GPU

## **2. Internal high-performance cluster ("Ažman HPC")**

16x 20-core Intel Xeon E5-2660v3 processors with 64 GB RAM

20x 16-core Intel Xeon E5-2650v2 processors with 32 GB RAM

20x 16-core Intel Xeon E5-2660 processors with 64 GB RAM

6x AMD Opteron 6128 with 16 GB RAM

30x 48-core AMD Ryzen Threadripper with 64 GB RAM and Nvidia GPUs

**TOTAL: ~4000 cores, 5.6 TB of RAM, 300 TB of storage**

**Combined computer power: 5 GFLOPS**

## **3. National supercomputing center (HPC Vega in Maribor, Slovenia), built in 2020**

BullSequana XH2000

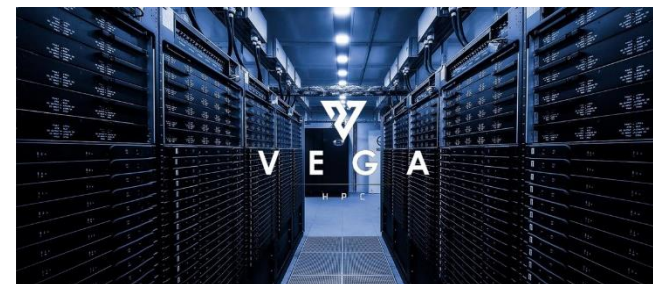
1920x AMD Epyc 7H12 (122.800 cores)

240x Nvidia A100

288 TB RAM

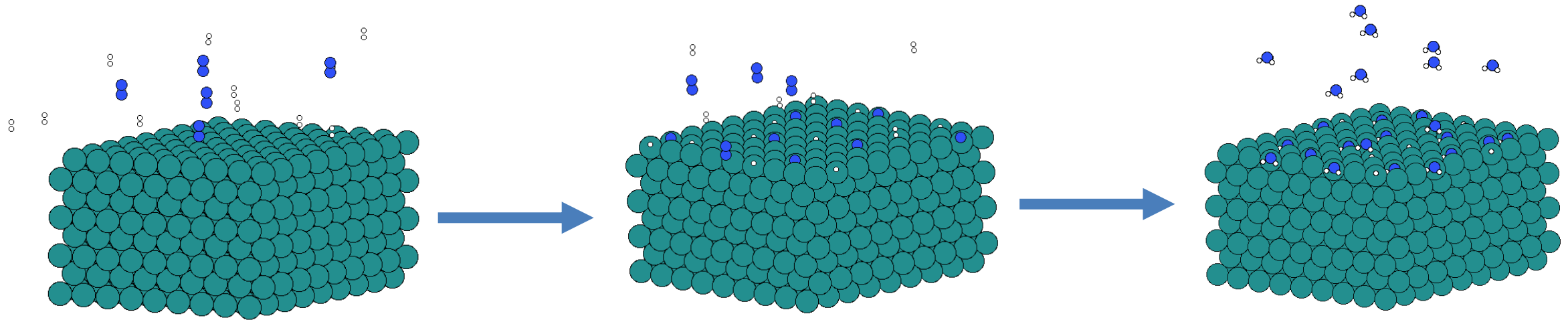
1 PB NVMe Lustre + 23 PB Ceph data storage



**Combined computer power: 10 PFLOPS (19<sup>th</sup> at the Top 500 list)**

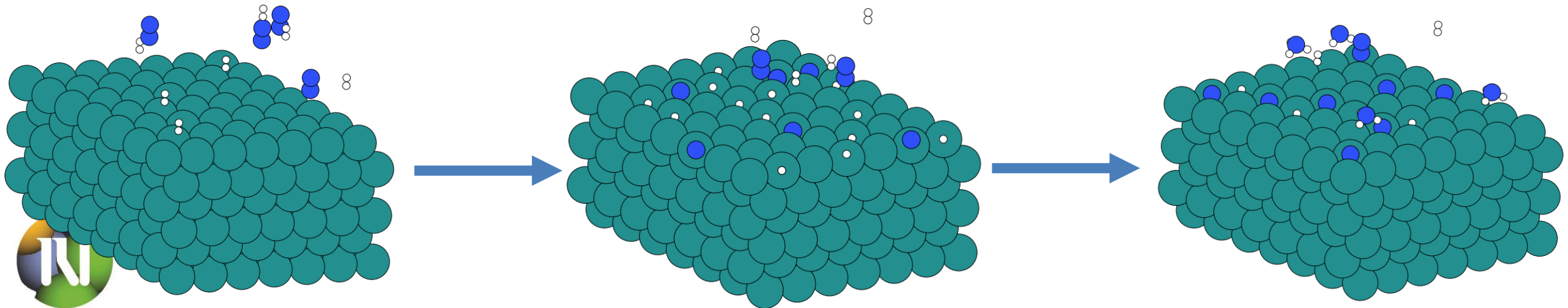




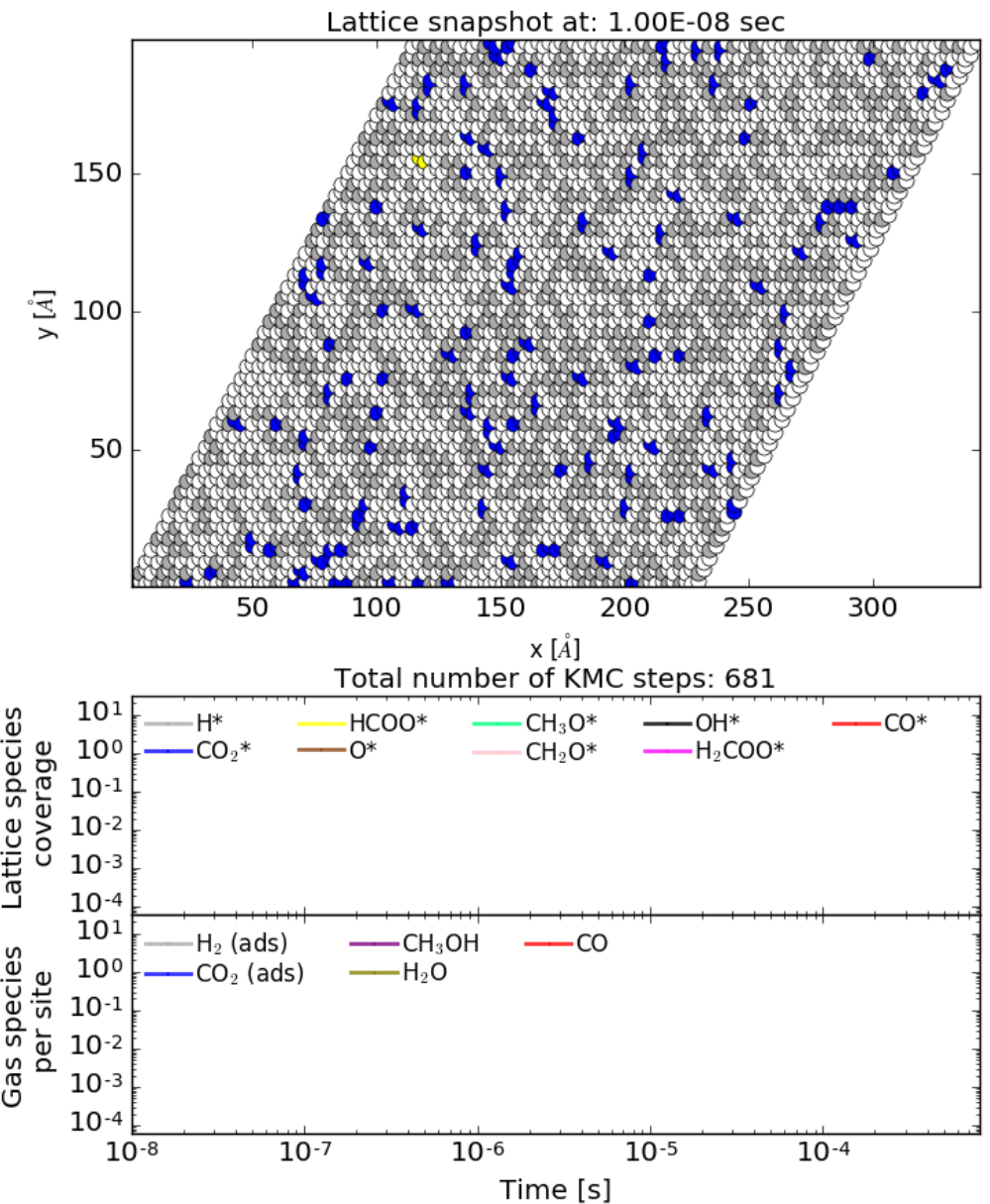
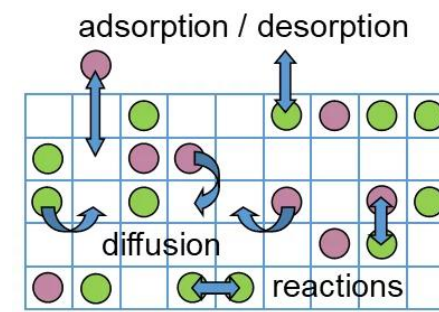
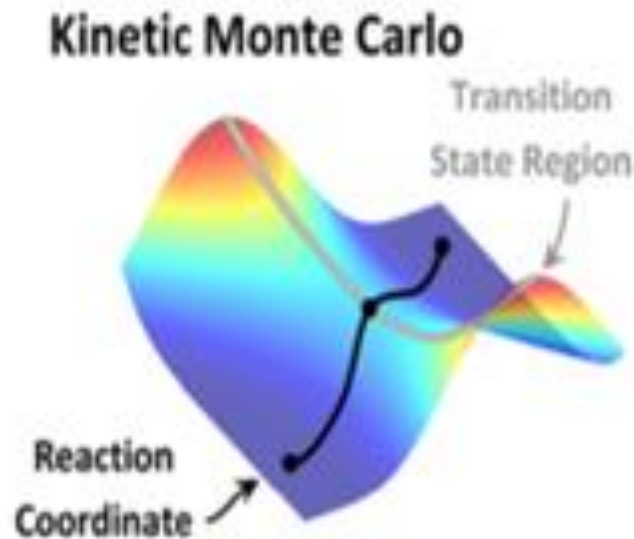
# AB INITIO MODELLING



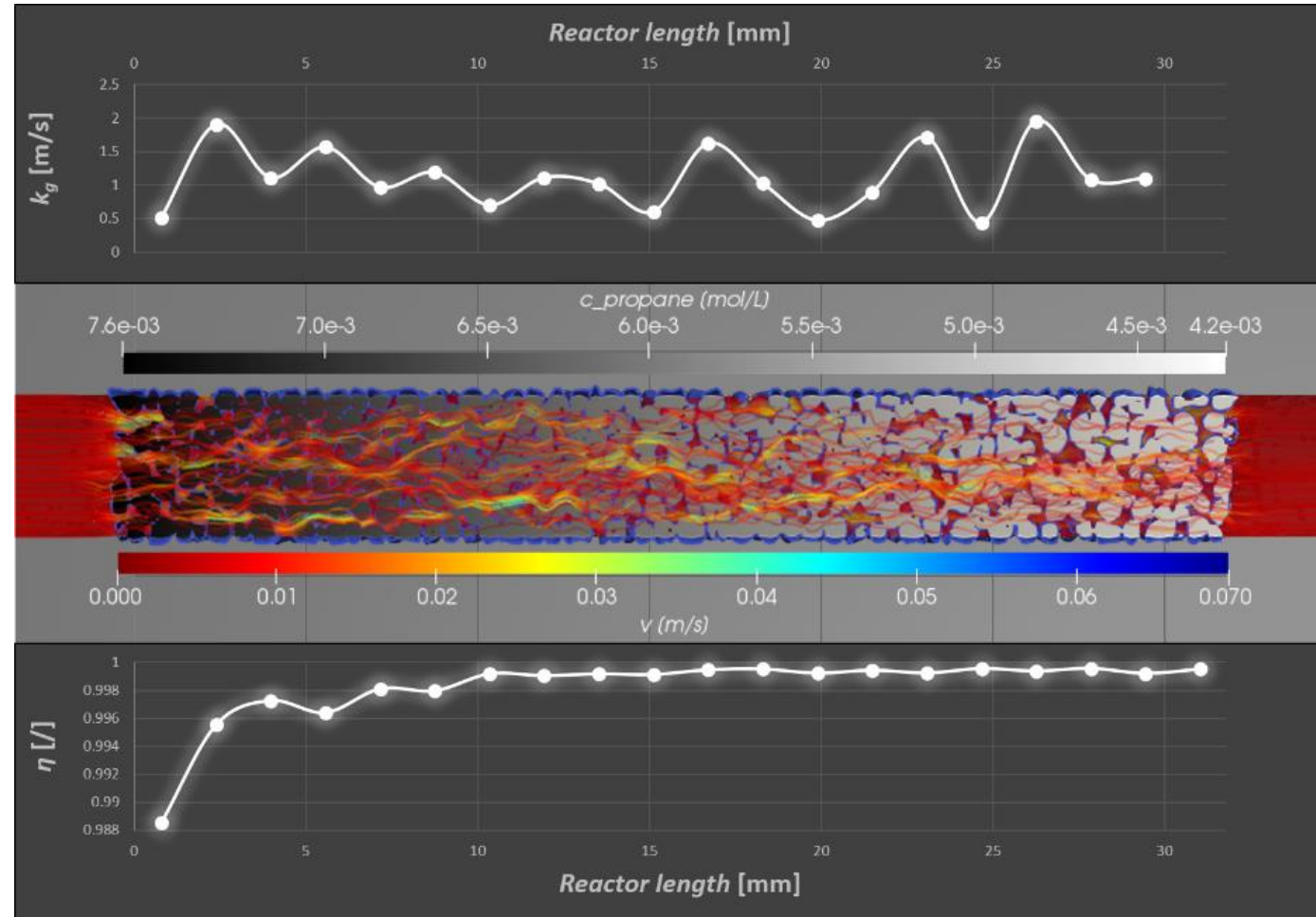
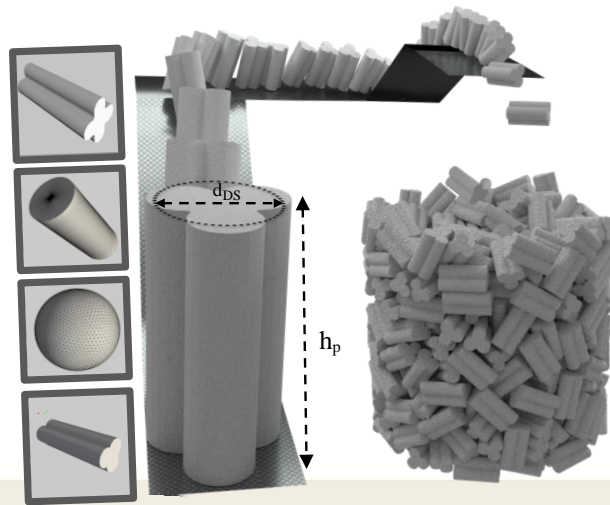
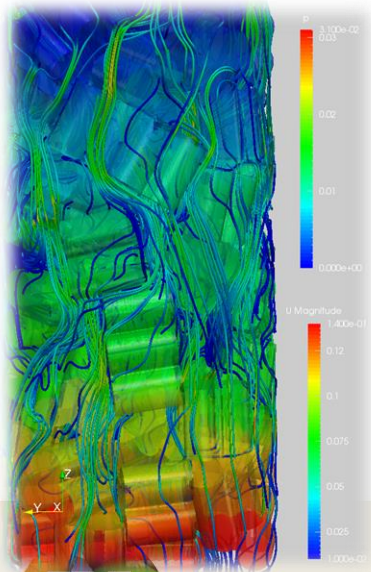
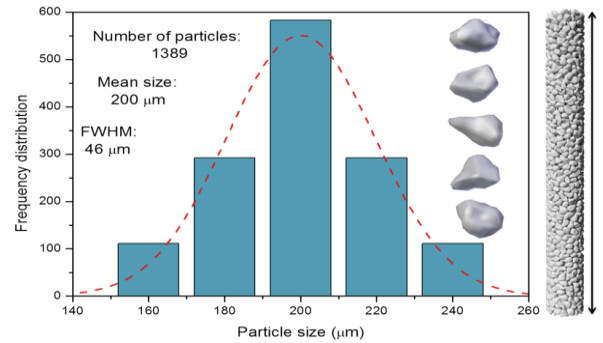
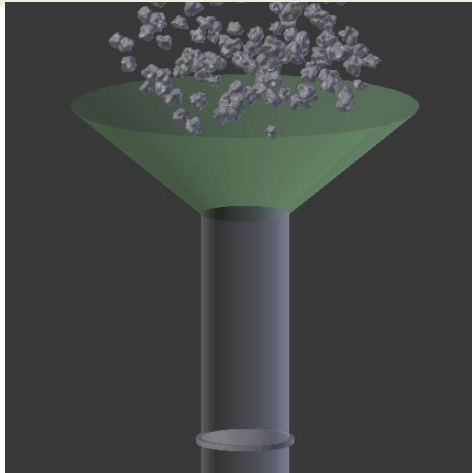
 - Nitrogen molecule  
 - Hydrogen molecule



# KINETIC MONTE CARLO



# MODELLING AT THE REACTOR LEVEL



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# ACKNOWLEDGEMENTS

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TotalEnergies



HRASTNIK1860



UPM



European  
Commission



BioSPRINT

BiZeolCat

CELEBio

CONVERGE

Carbon Valorisation in Energy-efficient Green fuels

FReSMe



MARIE SKŁODOWSKA-CURIE ACTIONS  
Research Fellowship Programme