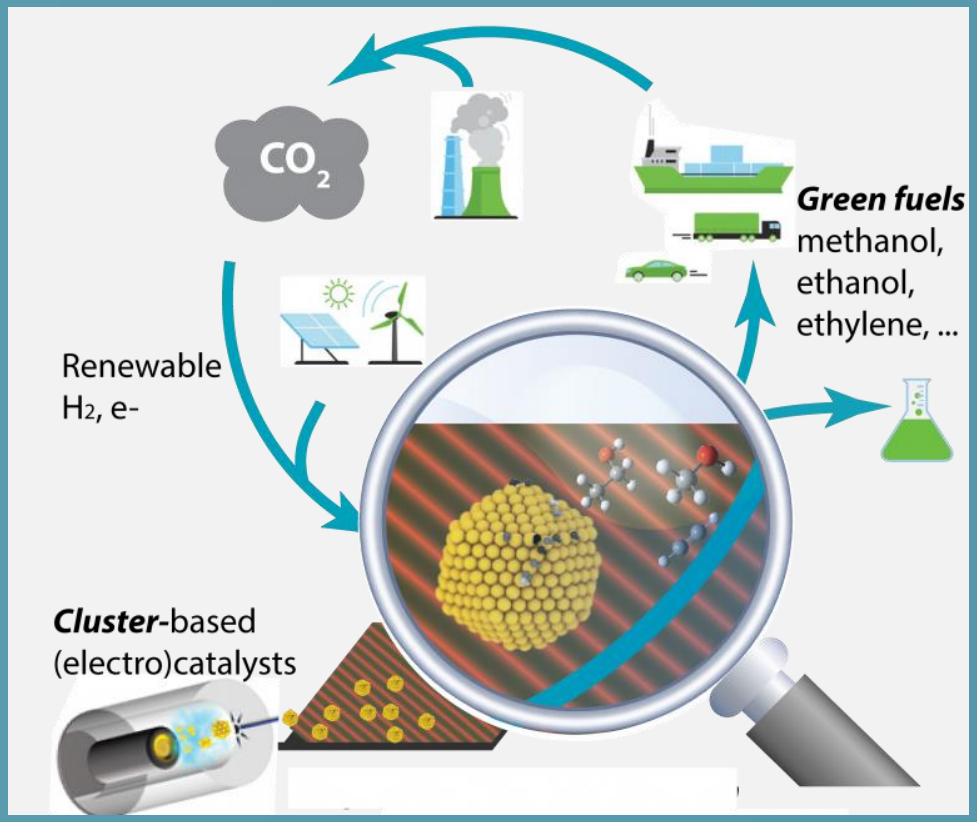
EUROPEAN TRAINING NETWORK
Novel catalysts for CO_2 Hydrogenation and Electro-reduction

Mid-Term Review
April 22, 2022, Budapest

Design, implementation and production upscaling of novel, high-performance, multimetallic cluster-based catalysts for CO_2 hydrogenation and electro-reduction (CATCHY)



- Conversion of CO_2 into methanol and C2 products
- (Bi)metallic clusters of few atoms to few nanometers
- Thermo- and electro-chemical route
- Complementary gas phase studies and computational modelling
- Catalysis-by-design approach; advances in atomic-scale understanding
- Interdisciplinary (physics, chemistry, and engineering) and intersectorial (universities, research institutes, companies) collaboration

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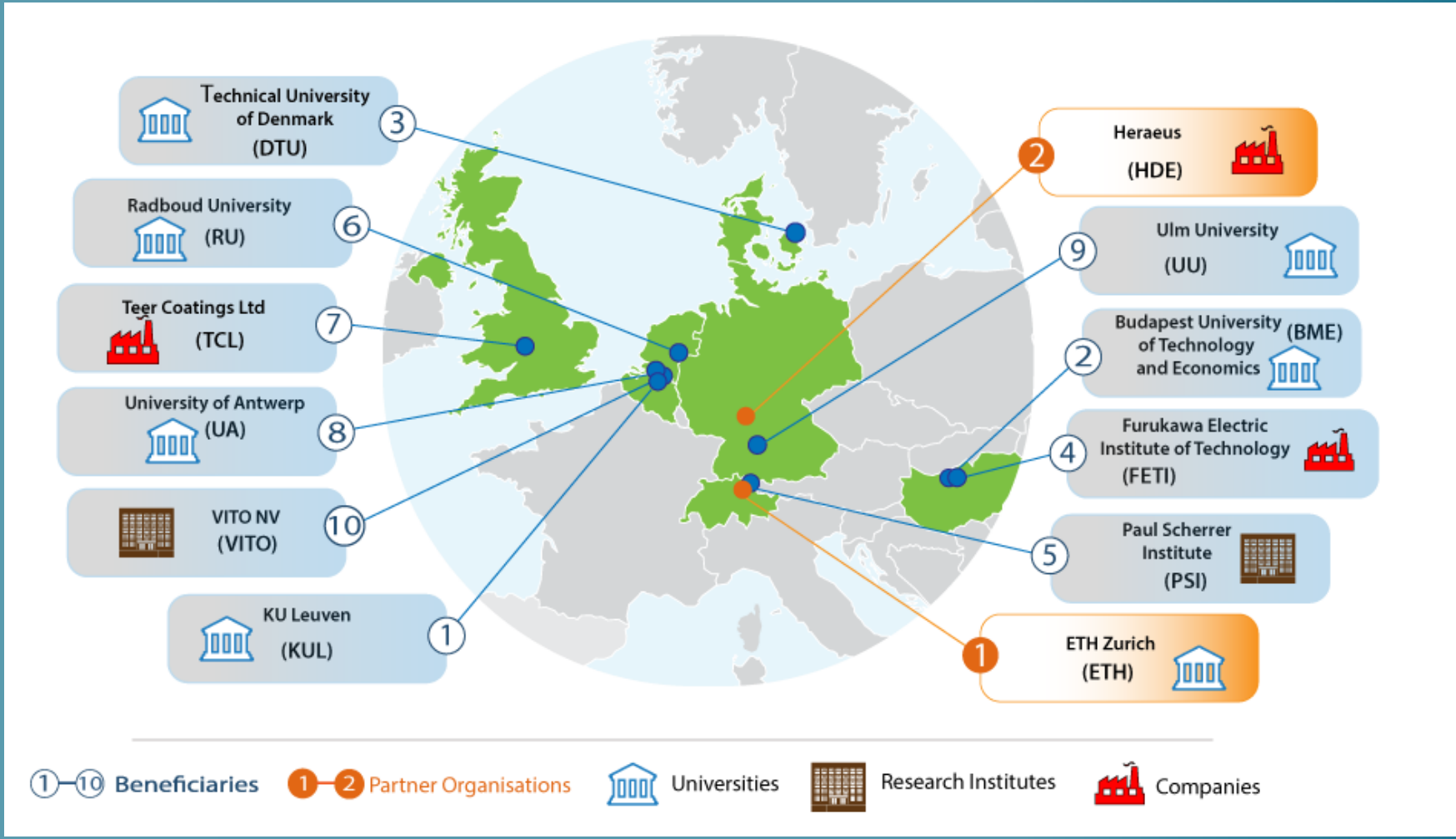

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Imran Abbas (KUL)

Joao Coroa (TCL)

Pavol Mikolay (UUlm)

Deepak Pradeep (RU)

Renata Sechi (FETI)

Bárbara Z. Yusti (BME)

Waqas Pervez (RU)

Dimitra Papamichail (KUL)

Sumant Phadke (PSI)

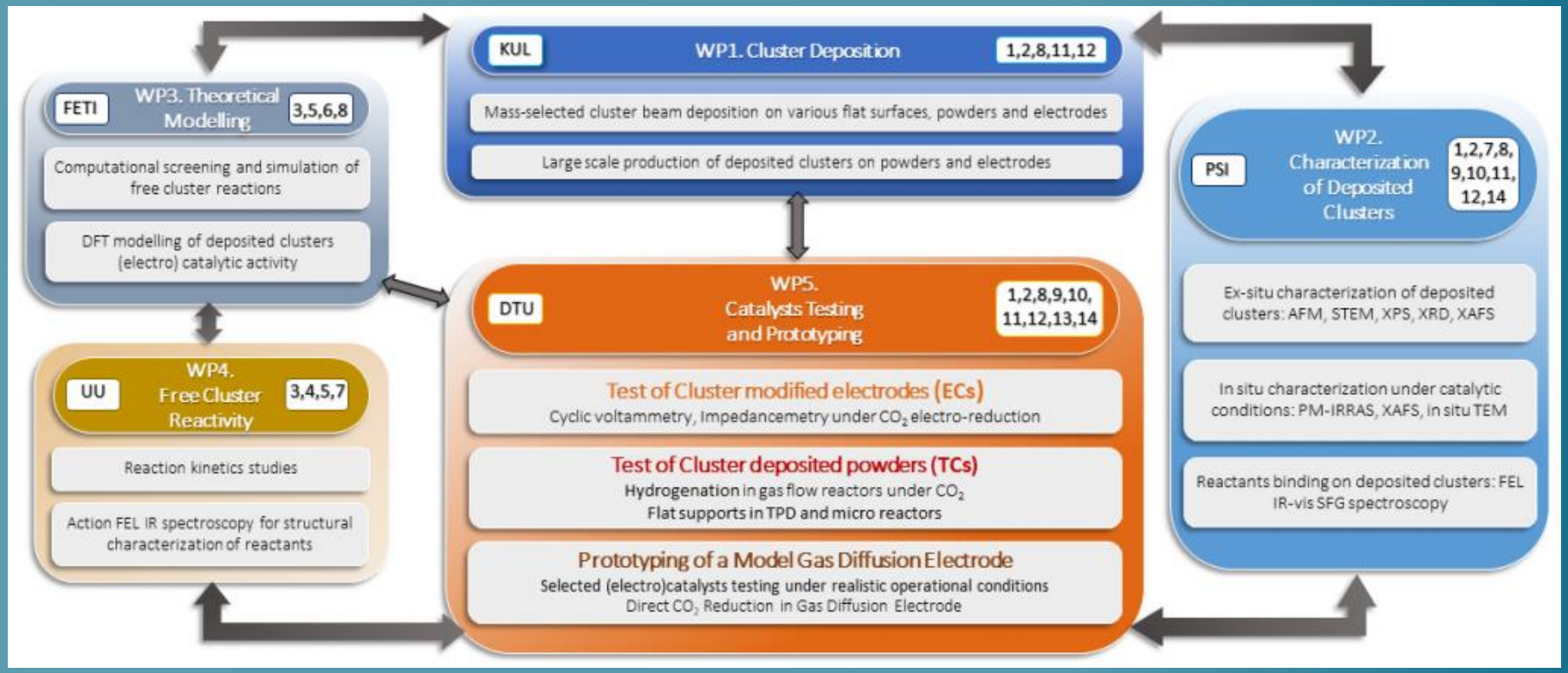
Deema Balalta (Uantwerp)

Filippo Romeggio (DTU)

Esperanza Sedano (DTU)

Wenjian Hu (VITO)

Maximilian Winzely (PSI)



- Production of mono- and bi-metallic clusters; mix noble, 3d and post-transition metals (WP1)
- Extensive characterization of their morphology, atomic structure and surface (ex and in situ) after deposition on different supports (WP2)
- Cluster investigations directly in the gas-phase (WP3) and theoretical modeling (WP4)
- Catalytic laboratory tests followed by the prototyping of the most promising thermo- and electro-catalyst for CO_2 conversion into valuable fuels and chemicals (WP5).

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State of affairs

WP1-5 – Scientific work packages

- Research activities for different WPs have started. Last month each WP leader organized scientific discussions (plan is to repeat this about twice per year).
- Status included in ESR presentations.

WP1 Cluster Deposition
Peter Lievens (KUL)

WP2 Characterization
Olga V. Safonova (PSI)

WP3 Theoretical Modelling
Tibor Höltzl (FETI)

WP4 Free Cluster Reactivity
Sandra M. Lang (UU)

WP5 Catalyst Testing and Prototyping
Christian D. Damsgaard (DTU)

- D1.1 Cluster deposition EC (KUL, TCL, DTU) – **submitted** Jan 2022
- D1.2 Cluster deposition TC (DTU, KUL) – **temporary report submitted** April 2022
- D1.3 Cluster production upscaling (TCL) – **in preparation** May 2022
- D2.1 in situ characterization TC (PSI) – **planned** November 2022
- D2.2 in situ characterization EC (PSI) – **planned** November 2022
- D2.3 in situ TEM characterization (UA) – **planned** November 2022
- D3.1 Theoretical charact. noble metal cluster EC (FETI) – **planned** May 2022
- D3.2 Theoretical charact. transition metal clusters (BME) – **planned** May 2022
- D3.3 Modelling reaction path free cluster (FETI) – **planned** September 2022
- D3.4 Modelling TC reaction path (BME) – **planned** September 2022
- D4.1 Mass spectra metal-oxide clusters (UU) – **submitted** March 2022
- D4.2 Reactivity free metal-oxide clusters (UU) – **planned** October 2022
- D5.1 Cluster-based TCs in gas flow reactors (DTU) – **planned** October 2022
- D5.2 Cluster-based ECs in electrochemical cells (DTU) – **planned** October 2022
- D5.3 Optimization cluster-modified electrode (VITO) – **planned** November 2022

Note: only leading institute mentioned, many report joint efforts
Note2: there may be delays wrt original plan

WP6 - Training

WP leader
Joost Bakker (RU)

Local training

- Local expert training through research (ongoing)
- Local skills training (ongoing)
- Interdisciplinary and intersectorial secondment programme (ongoing)

  There are in total 38 secondments (76 months) planned, of which 6 secondments (12 months) were done or are ongoing. 12 others are planned in 2022.

  Some secondments have been shifted in time due to late recruitment, practical concerns, or better fit with ESR's training plans (see prelim. D6.7)

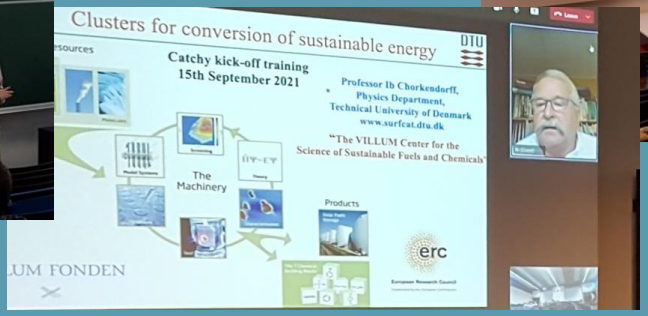
  Reminder: secondment plan before and report after (template on intranet)

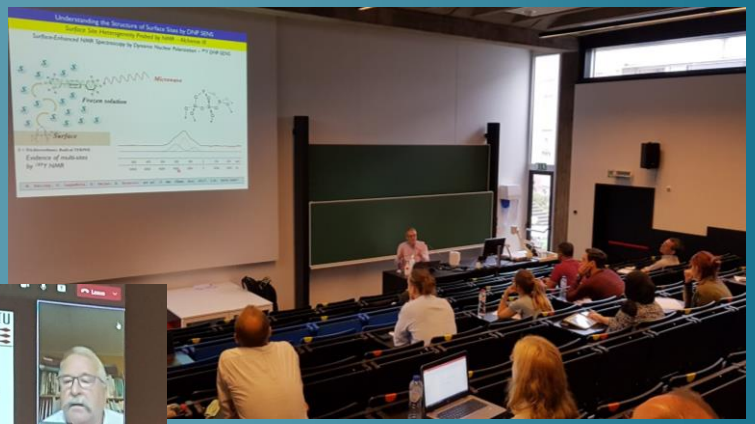
Network wide training

- 7 planned network wide training events (NWTEs) of which two took place and one more will be organized in 2022. The NWTEs combine scientific and skills trainings and foster cross-disciplinary interactions.

NWT1 – Kick-off training (September 2021, Leuven, Belgium)

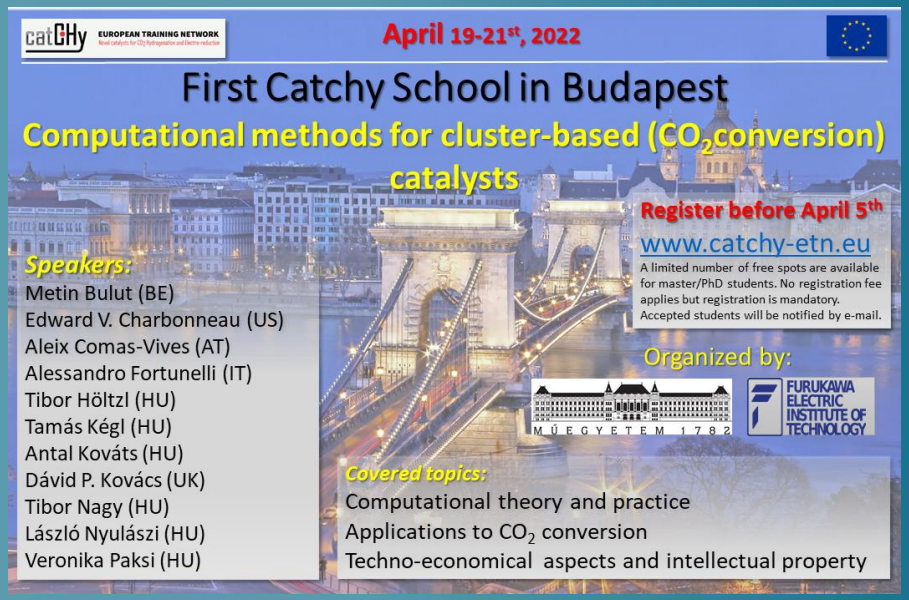
- *S&T training*: state-of-the-art on thermo- and electro-catalysis for the capture and conversion of atmospheric CO_2 into added-value fuels. 8 lectures, including 5 invited experts outside the Catchy network.
- *Skills training*: scientific communication, data management, research integrity, and diversity in research teams. 4 lectures given by 5 invited speakers (KU Leuven and VITO)
- 28 participants including 8 external PhD students.





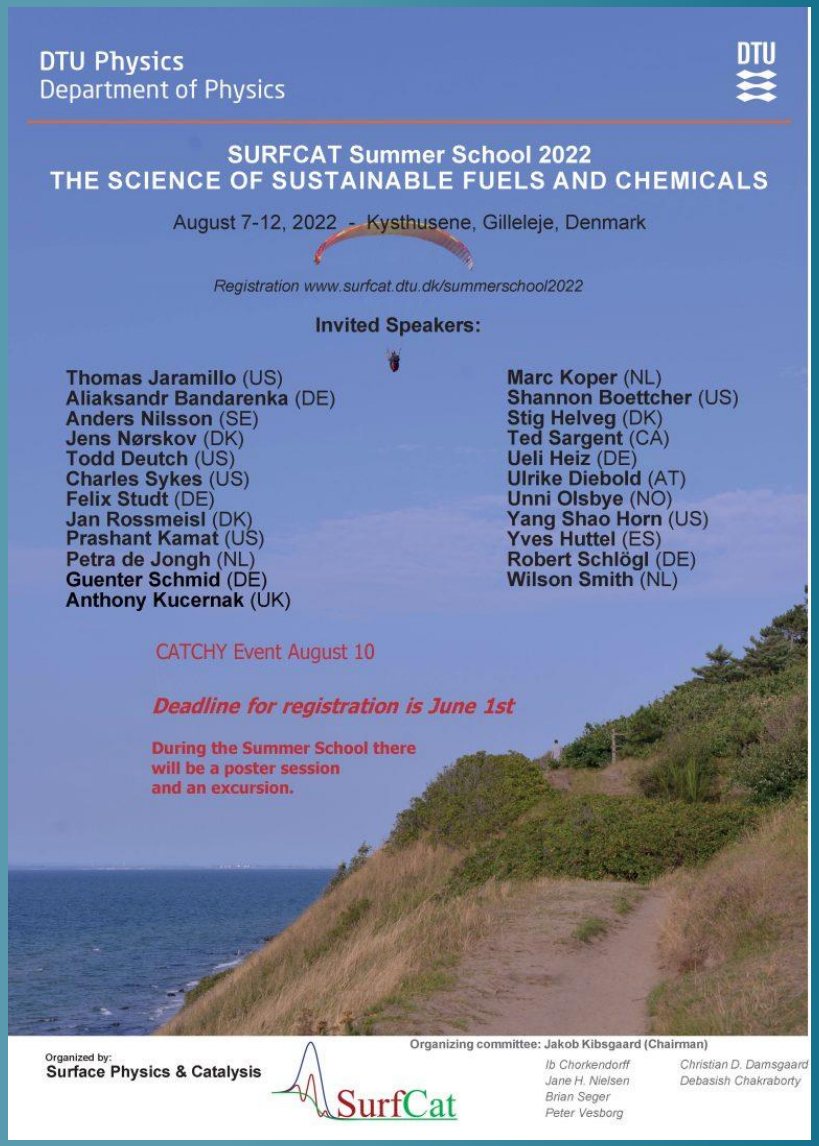
NWT2 – School on Computational methods for cluster-based catalysts (April 2022, Budapest, Hungary)

- *S&T training*: Introduction to computational chemistry and its applications to cluster-based CO_2 conversion catalysis. 8 lectures of which 5 delivered by invited experts.
- *Skills training*: practical training in computational modelling, techno-economical aspects of CCU, lecture on gender in science, and 3 company presentations. 6 presentations among which 3 speakers from outside the Catchy network.
- 49 participants, including 25 external master and PhD students.



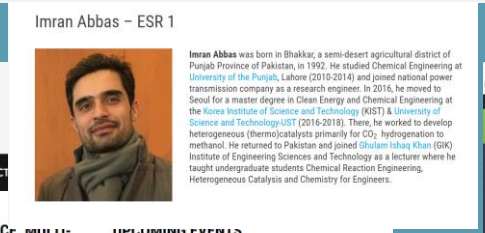
NWT3 – SURFCAT Summer School 2022: Science of Sustainable Fuels and Chemicals (planned August 7-12, 2022, Gilleleje, Denmark)

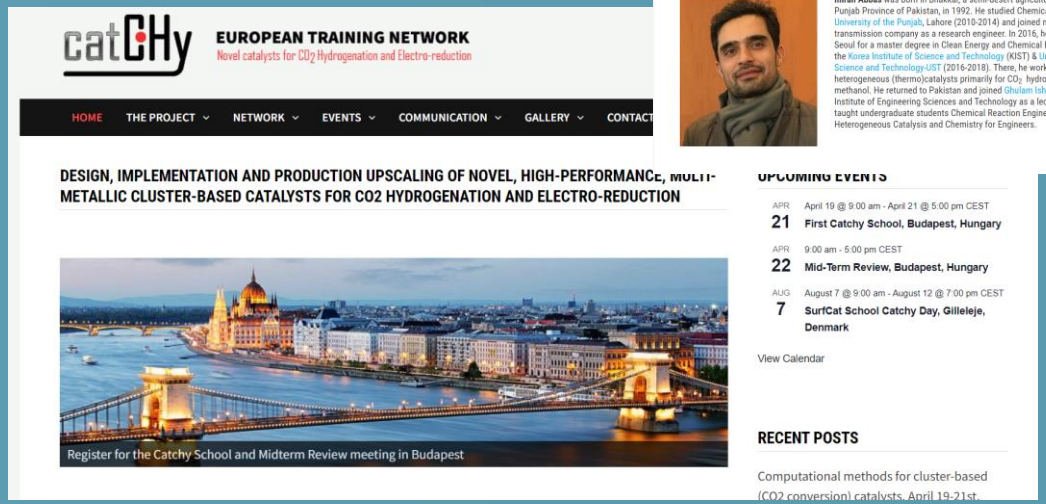
- *S&T training*: School on catalysis, featuring internationally known invited speakers with complementary backgrounds in the theoretical and experimental aspects of photocatalysis, electrocatalysis, and heterogeneous catalysis. Experts will present a span of lectures from basic concepts in catalysis and characterization techniques to cutting edge research with special focus on sustainable pathways to fuels and chemicals.
- Catchy Event with visit at Haldor Topsoe and lab tour DTU Physics

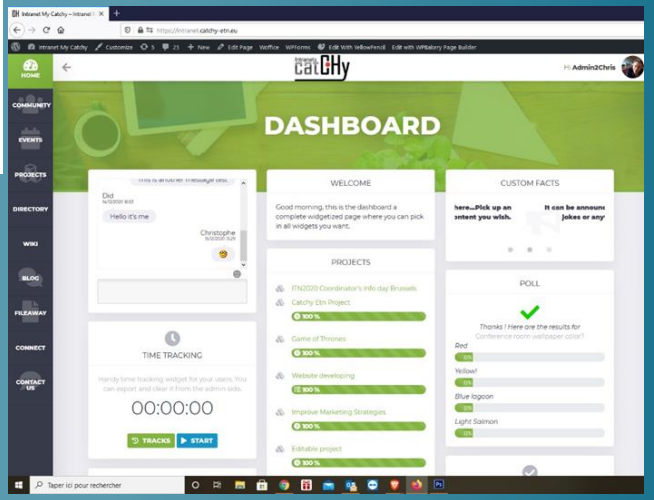


WP7 - Dissemination, Exploitation, Communication, and Outreach

- Website external (incl. ESR pitch) and intranet (done Oct 2021, D7.1 and D7.3)
- Communication and Dissemination plan (done March 2021, D7.2)
- IPR policy (done, June 2021, D7.4) → IP manager Debasish Chakraborty
- Catchy Twitter (Imran), LinkedIn (Esperanza), Instagram (Deema) pages
- Microdocs (**planned – July 2022! Action – all ESRs**)
- First papers (**planned** – Dec 2022)





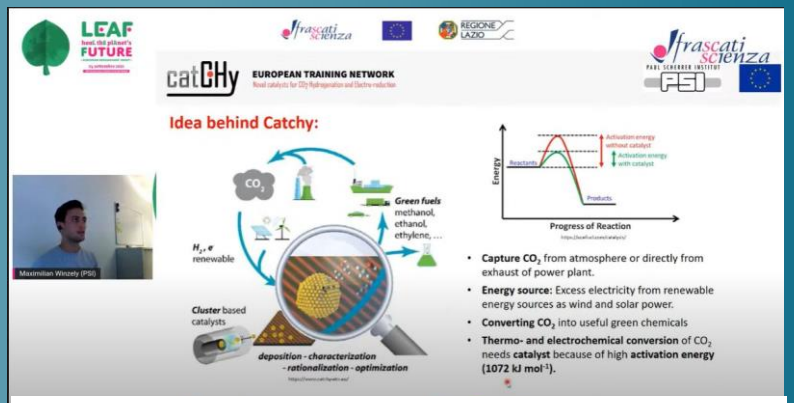


WP7 - Dissemination, Exploitation, Communication, and Outreach

Outreach:

- Some beautiful outreach activities took place, other are planned (cf. microdocs)
- keep record (inform **Didier**) about all outreach / dissemination activities (incl. conference contributions/papers) in the context of the Catchy project (**Action – all**) **IMPORTANT**

Renata – Blowing CO_2 away (European Researchers Night @BME)



Maximilian - European Researchers Night @ PSI and Frascati Laboratory

WP8 – Project management

WP leader
Ewald Janssens
(KUL)

- Supervisory board (established Jan 2021, D8.1)
- Consortium agreement (done Feb 2021, D8.2)
- ESR positions advertised (done Feb 2021, D8.3)
- Data management plan (done, April 2021)
- Personal Career Development Plan (done, Sep 2021 – update April 2022, D8.5)
- Progress Report (submitted Jan 2022 D8.6) and Project check (**ongoing**, D8.7)

Personal Career Development Plan

PCDP

Marie Skłodowska-Curie Actions

ESR information			
ESR#	<Last Name>	<First Name>	Title
Employer <Institution Name>		Academic institution (if different) <Institution Name>	
Supervisor			
Main promotor	<Last Name>	<First Name>	Title
Academic promotor	<Last Name>	<First Name>	Title
Project breakdown [100%]			
Main research <xx%>	Secondment <e.g. 4/36M=11%>	Training & Mentoring <xx%>	Dissemination & Outreach <xx%>
Project title	<My project>		WP#
Project milestones *(e.g. simulations, experiments, publication, conferences, defense, ...)*			Timeline
• <milestone 1> • <milestone 2> *Formulate the milestones through which you will evaluate your own progress.* *These may include but are not limited to the 'project milestones' from the Grant Agreement Annex 1. Consider research-related milestones (e.g. performing a specific experiment, reaching a specific precision on an output, ...) as well as practical milestones (e.g. 9-month doctoral evaluation, participation in an international conference, defending your thesis, ...)* *The ESRs are stimulated to consider how their milestones may contribute to overall CATCHY research deliverables and milestone (sections 1.3.2-4, p77 ff in GA)*			<mm/20xx> <mm/20yy>

Reminder: PCDP to be updated yearly (**action all**)

Milestones

- MS1 – pre-recruitment (done, Feb 2021)
- MS2 – recruitment of 14 ESRs completed (done, Dec 2021)
- MS3 – 14 PCDP written (done, Feb 2022)
- MS4 – 14 Doctoral guidance committees (still do be approved by SB)
- MS5 – Midterm meeting held (now)
- MS6 – Upscaled cluster production WP1 (**TCL**, **target** May 2022)
- MS7 – 1st publ. in situ characterization WP2 (**PSI**, **target** Dec 2022)
- MS8 – 1st publ. theoretical chacarterization WP3 (**FETI**, **target** Dec 2022)
- MS9 – 1st publ. free cluster reactivity WP4 (**UU**, **target** Dec 2022)
- MS10 – 1st publ. CO_2 conversion WP5 (**DTU**, **target** Dec2022)

Risks / threads

- R1: Delay in recruitment (**materialized**)
  - see following slide on Covid Impact on Catchy
- R2: Key staff leaving the project - no sign that risk might materialize
- R3: Lack of cooperation from a participant - no sign that risk might materialize
- R4: Conflict about IP: no issues yet
- R5: PhD absorbed if funding stops after 3 years: too early to evaluate

Covid Impact on Catchy

- Severe impact on the recruitment process of ESR11@DTU: postponed by 6 months.
  - ✓ As a consequence ESRs 1, 9 and 10 have postponed their secondments to DTU in order to be able to allow interaction
  - ✓ Induced significant delay on D1.2 deliverable
- Large fraction of ESRs contracted Covid and/or had to quarantine.
- Other delays of 4 to 6 months in ordering scientific equipment (still ongoing).
- A 6-month extension of the duration of Catchy would allow the completion of the PhD of ESR11 and several other ESRs.


Thanks for your attention