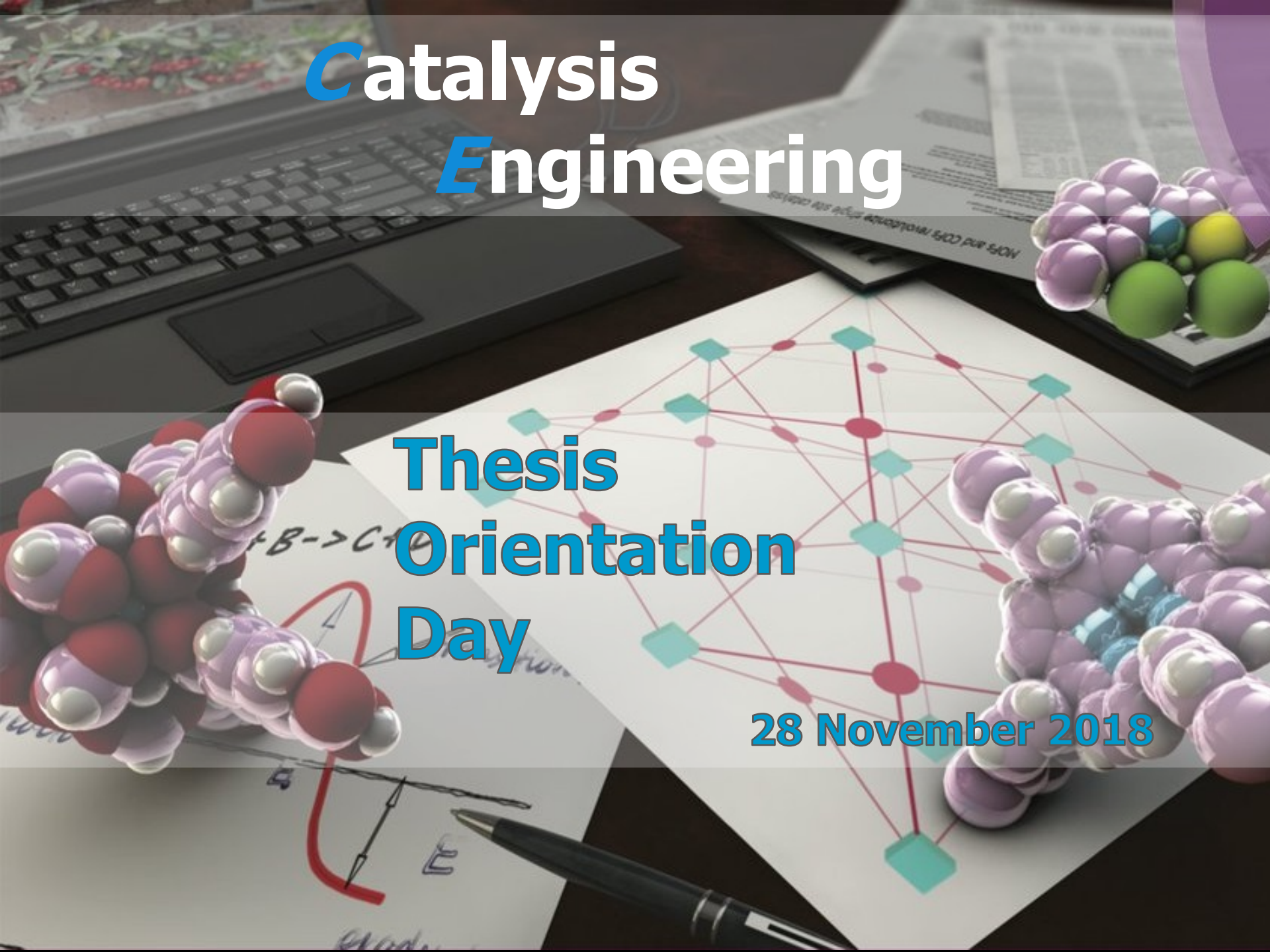


Catalysis Engineering

The background features a dark desk with a laptop on the left, several papers scattered across the center, and a black pen in the bottom foreground. Three 3D molecular models are visible: one on the left with red, purple, and white spheres; one on the right with purple, green, and blue spheres; and a smaller one in the top right corner with purple, blue, and yellow spheres. A network diagram with red lines and cyan and red nodes is overlaid on a paper in the center.

**Thesis
Orientation
Day**

28 November 2018

Catalysis Engineering



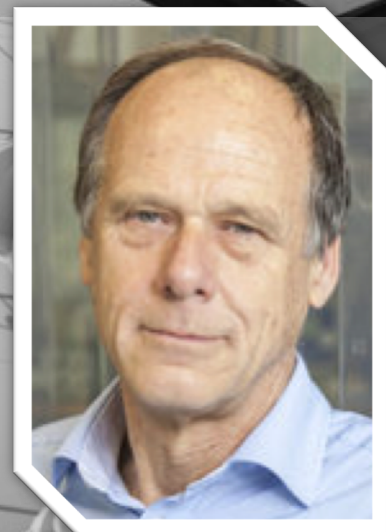
Atsushi Urakawa



Freek Kapteijn



**Monique
van der Veen**

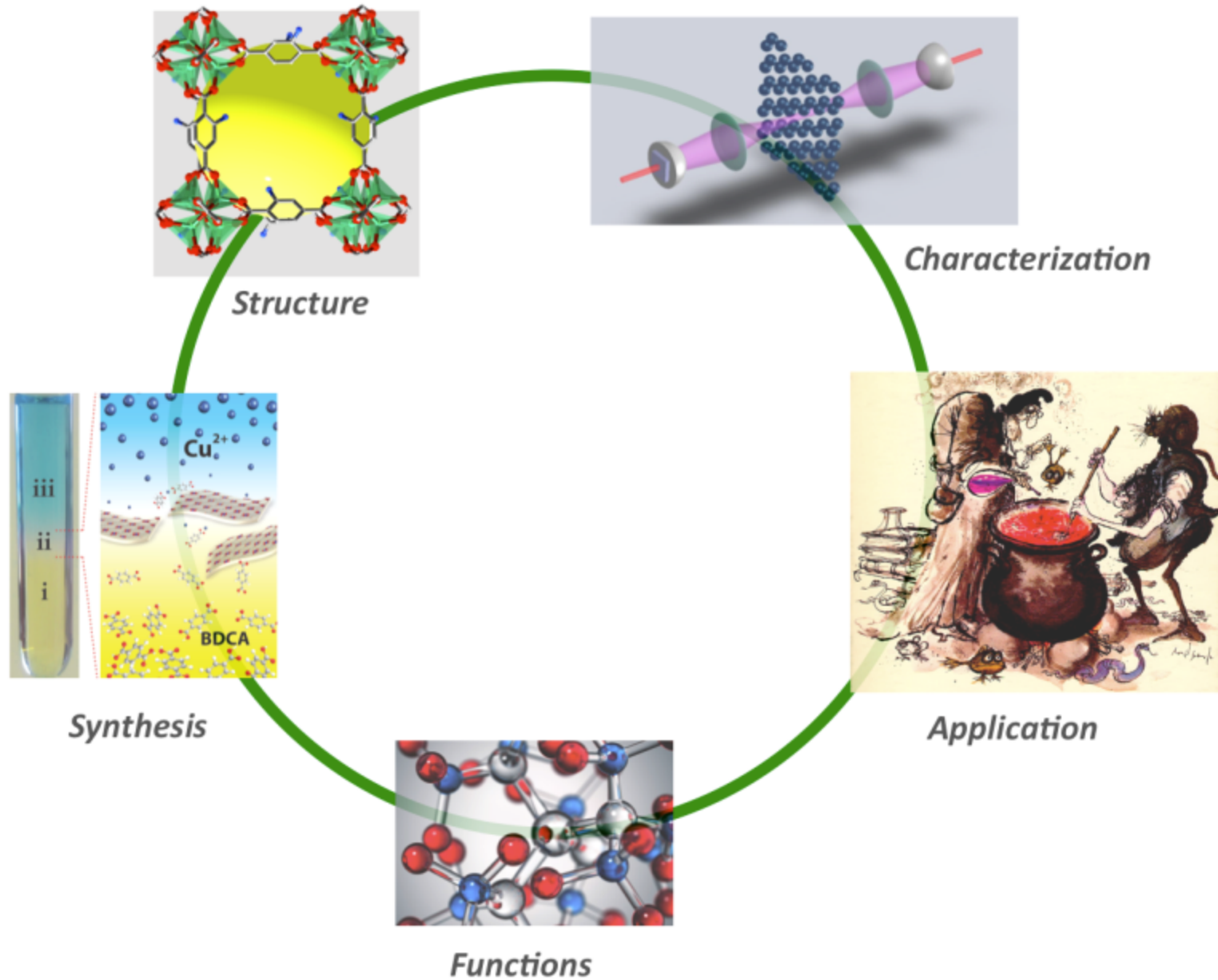


Michiel Makkee

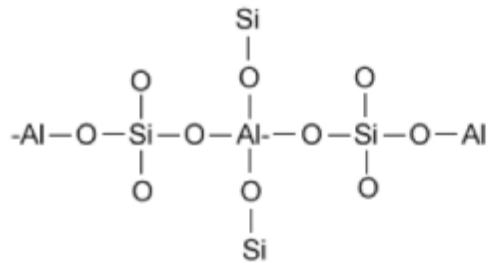
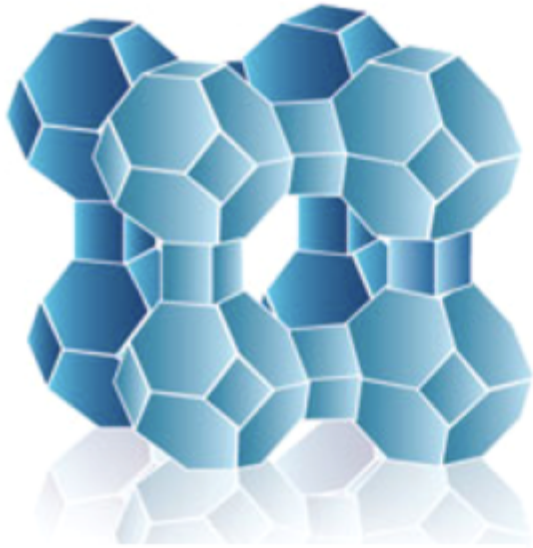


Catalysis
Engineering

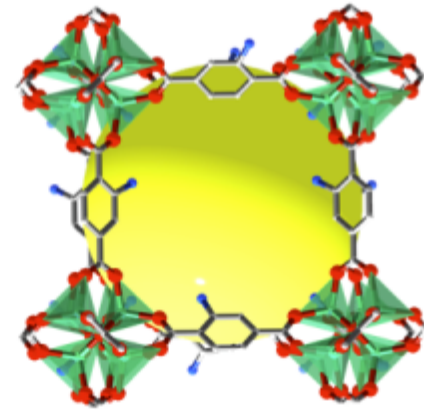
Our philosophy



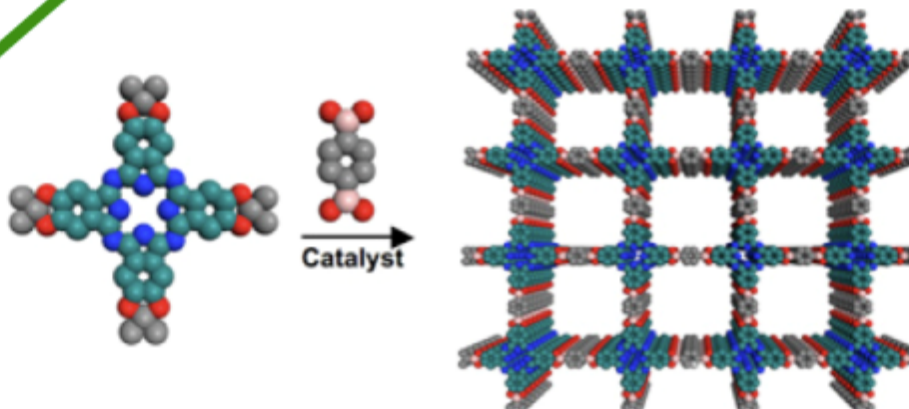
Zeolites



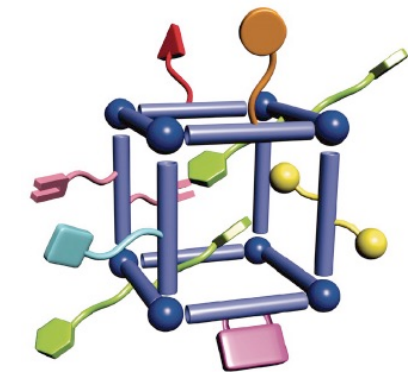
MOFs



Structured polymers

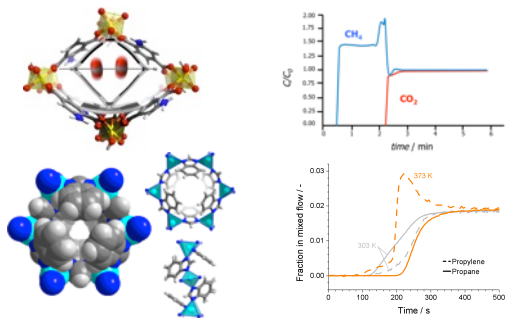


Advanced Functional Materials

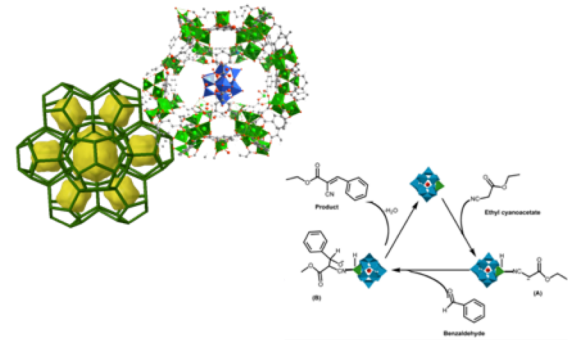


Catalysis Engineering

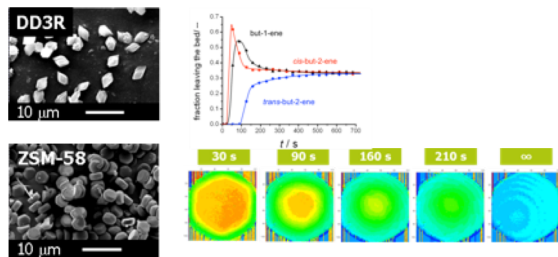
MOF separation



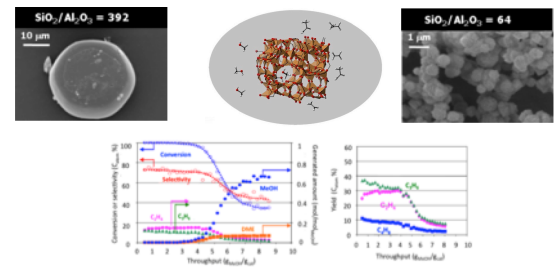
MOF catalysis



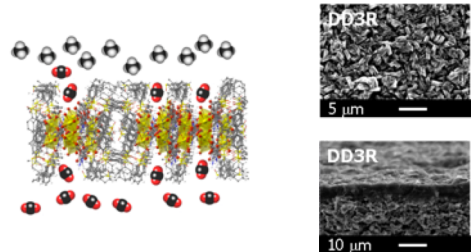
Zeolite diffusion



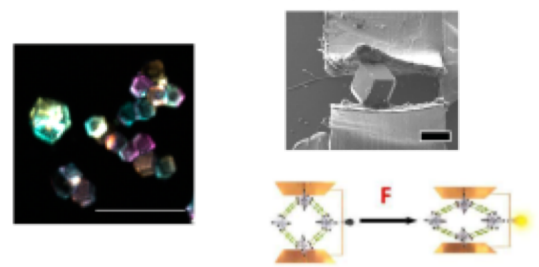
Zeolite catalysis



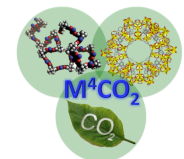
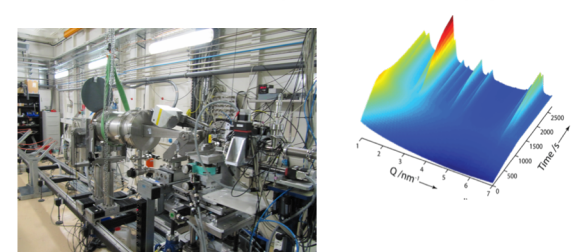
Membranes



MOF electronic applications



Advanced spectroscopy

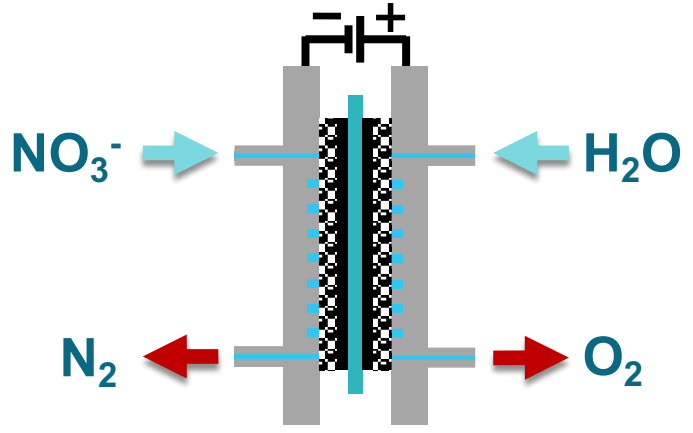


Catalysis Engineering

The background features a blue-tinted collage of scientific and engineering elements. On the left, a laptop keyboard is visible. In the center, there are several sheets of paper, one of which displays a complex network diagram with nodes and connecting lines. To the right, there are several 3D ball-and-stick molecular models of various sizes and shapes. A pen is also visible in the lower foreground.

Theme 1: Heterogeneous catalysis for sustainable generation of energy and chemicals

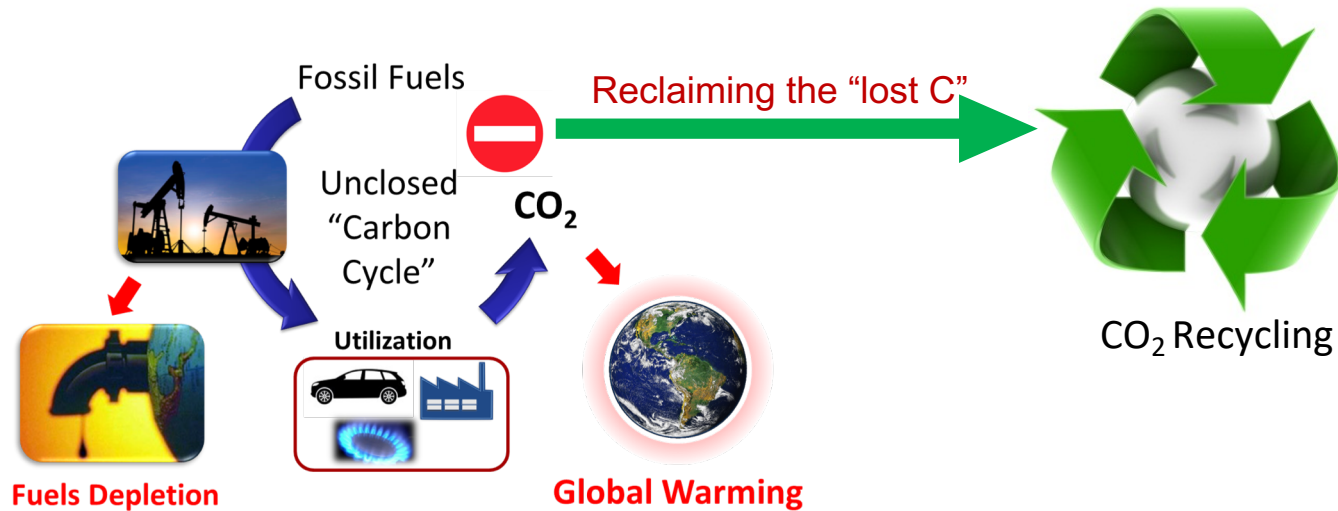
Electrochemical NO₃⁻ reduction in a PEM Electrolyzer



- You will learn:**
- To synthesize heterogeneous electrocatalysts
 - To perform catalyst characterization
 - To assemble and operate a PEM electrolyzer cell
 - To optimize reaction parameters in order to obtain the best activity and selectivity towards NO₃⁻ reduction

For more information contact Sorin Bunea (s.bunea@tudelft.nl)

Development of catalytic CO₂ conversion processes



Target projects

- Development of innovative characterization methods/tools for *in situ/operando* studies
- High pressure catalytic CO₂ hydrogenation to industrially important chemicals & fuels
- Process optimization and catalytic activity evaluation using high pressure micro-reactors
- New catalytic material development using novel synthesis methods

Keywords :- heterogenous catalysis, micro reactors, online gas chromatography, high pressure, inorganic material synthesis, space and time resolved approaches, process optimization, spectroscopy

Found interesting?

Contact Dr. Atul Bansode (A.B.Bansode@tudelft.nl) for more information

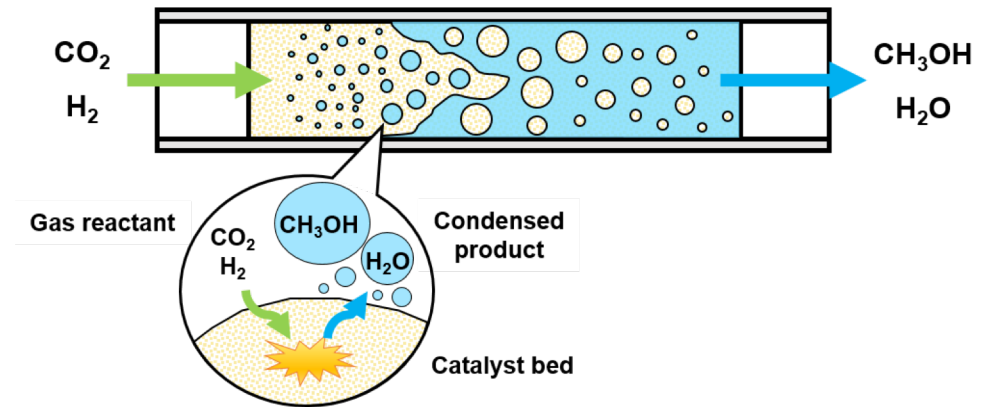


High-pressure CO₂ hydrogenation to methanol

(up to 400 bar)

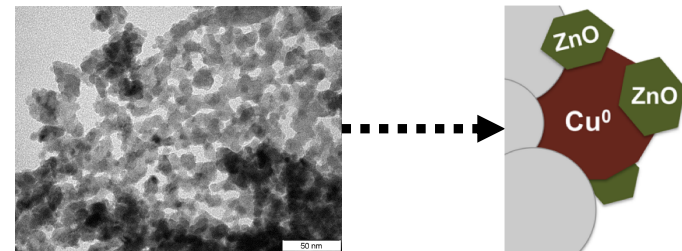
Why using high pressure?

We use high pressure to increase productivity and overcome one-phase chemical equilibrium by *in situ* phase condensation and separation of products.



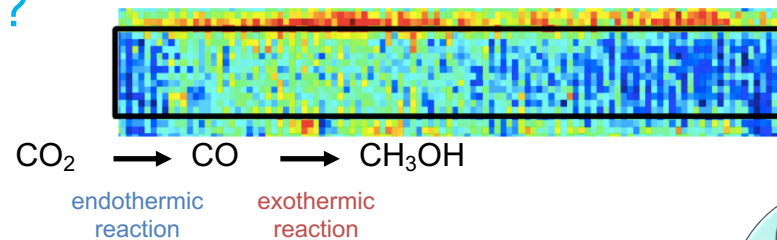
How do we make reaction faster?

Commercially, Cu/ZnO/Al₂O₃ catalysts are used. We developed a preparation technique for such catalysts with high Cu dispersion and intimate contact between Cu and ZnO.



What do we eventually want to see?

We want to see the catalyst bed under working conditions. With an IR camera, we observed temperature gradients originated from multi-step reaction pathway. The reaction mechanisms could be further investigated by IR spectroscopy.



Heterogeneous catalysis - In situ/Operando analysis

Investigate the catalyst in real operation conditions

Space and time resolution of the information



TOPIC

Methane activation to valuable chemical/fuels

Partial Oxidation
Dry Reforming

GOALS

Fundamental steps of the reactions
Catalyst properties controlling activity/selectivity

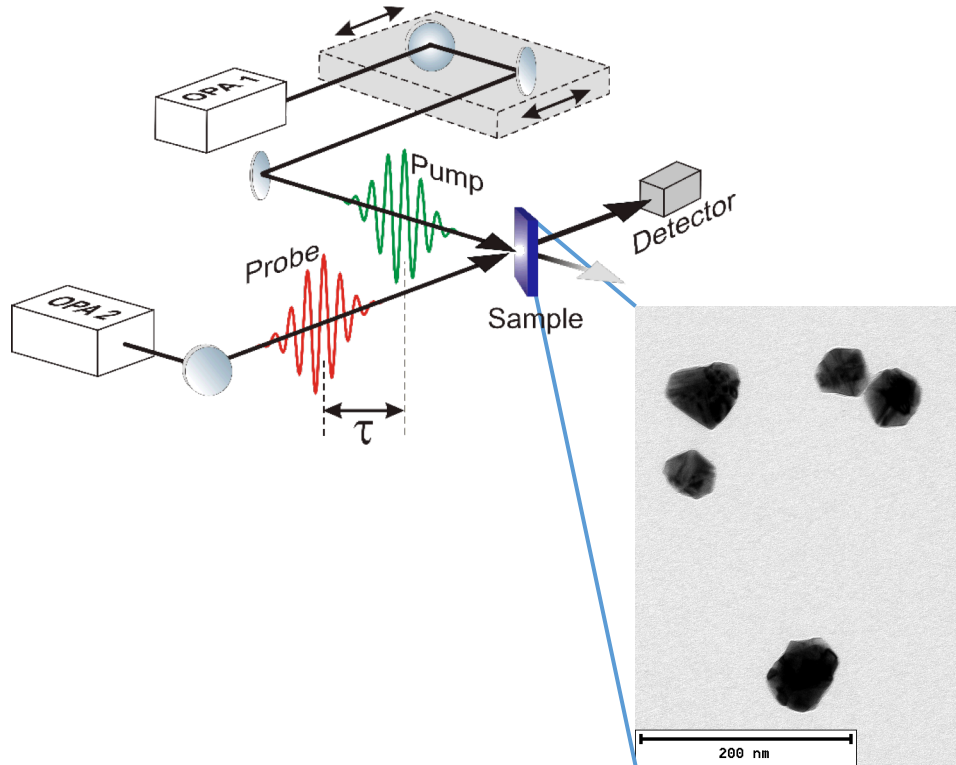
TOOLS

IR spectroscopy, Mass Spectrometry, Gas Chromatography, etc.
Data processing and automation (Matlab)



For more information contact: d.pinto@tudelft.nl

Ultrafast spectroscopy for reaction dynamics



Plasmonic nanoparticles

Femtosecond light pulse \rightarrow

Nanosecond heating \rightarrow

Study reaction dynamics

Research areas

Nanoparticle synthesis

Time-resolved spectroscopy

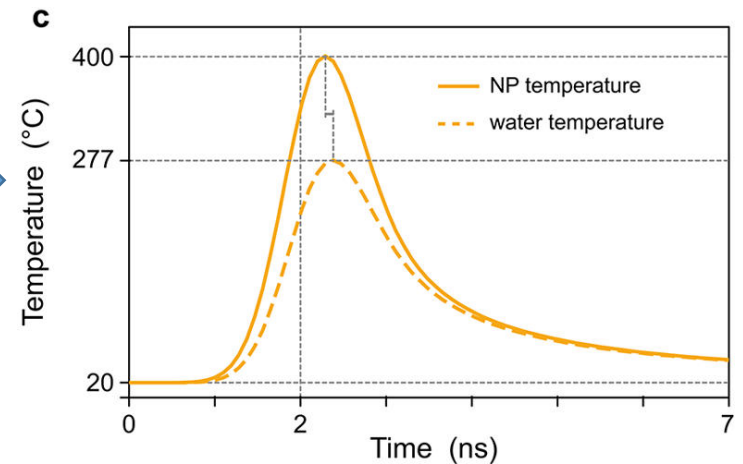
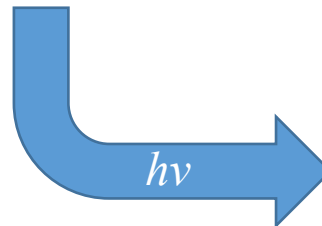
Reaction dynamics



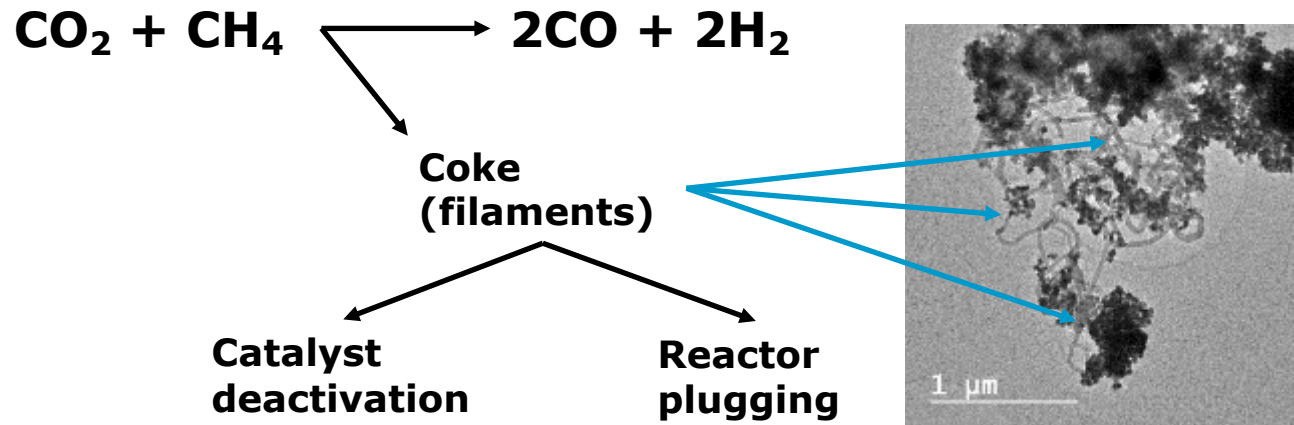
Contact

Han Mertens

j.c.j.mertens@tudelft.nl



Deactivation of methane dry reforming catalysts



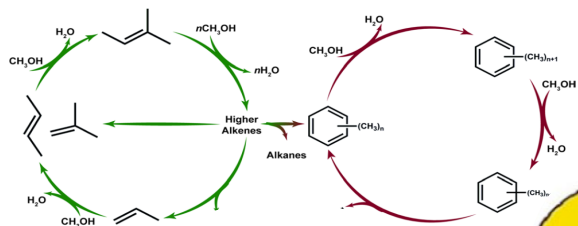
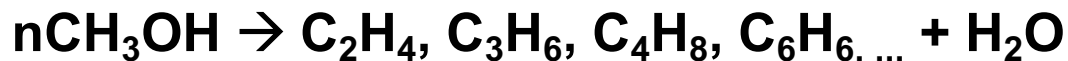
Projects:

- Studying the impact of different catalytic promoters
- Optimizing the pre-treatment and reaction procedures

Typical activities: Catalyst synthesis and testing, temperature programmed analyses, electron microscopy, spectroscopic techniques

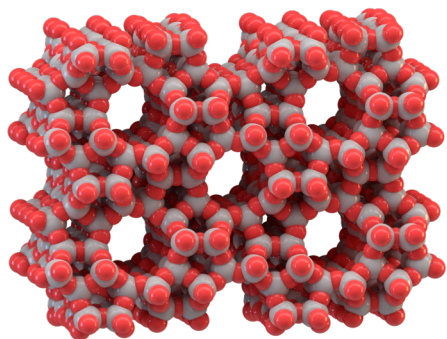
For more information, please contact Robert Franz: r.p.m.franz@tudelft.nl

Investigation of Non-commodity Zeolite Frameworks for MTH reaction



Targets:

- ❖ Highly selective to favoured products
- ❖ Stable – no deactivation

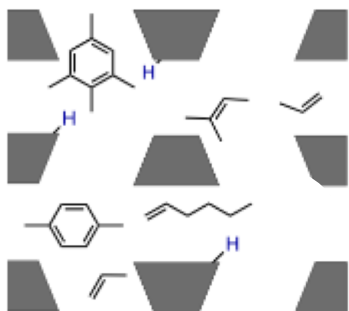


Main activities:

- Test MTH catalytic process by varying working conditions
- Figure out the structure-performance correlation
- obtain mechanistic insights of the coking process



For more info: Chuncheng Liu
C.Liu-6@tudelft.nl



Catalysis Engineering

Theme 2: Nanoporous materials for emerging applications

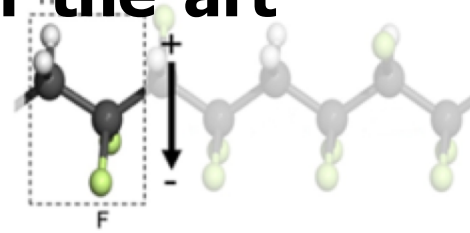


MOFs: The first tuneable ferroelectrics



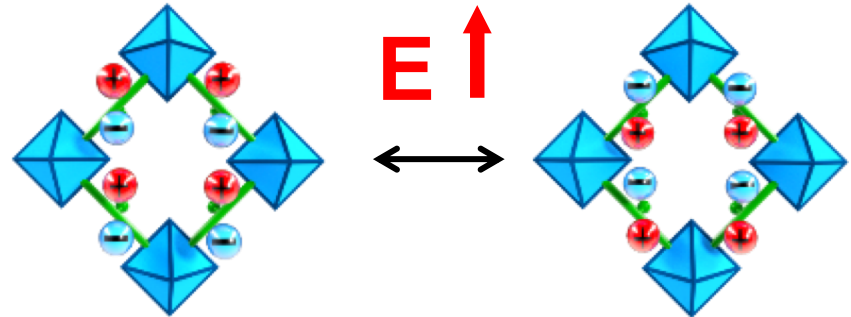
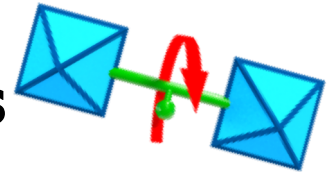
Challenge

State-of-the-art



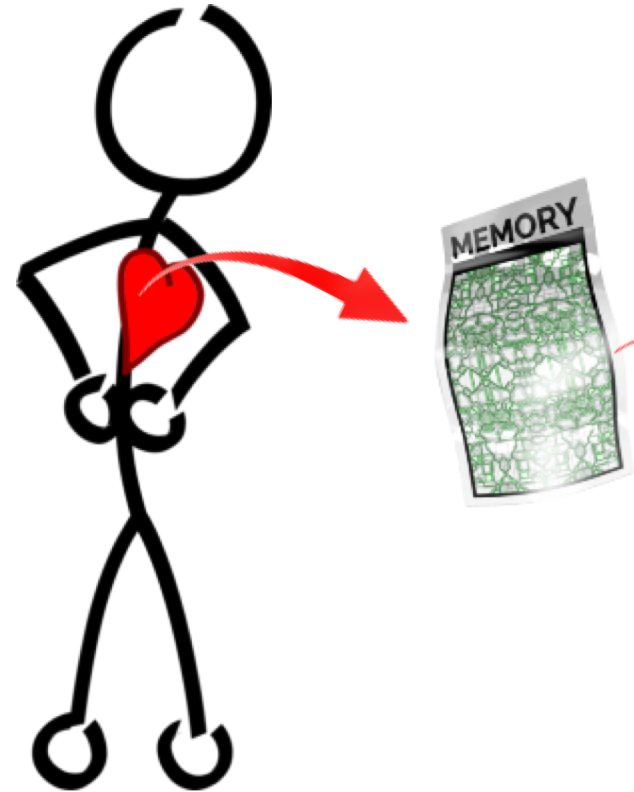
Innovative Solution

Polar MOFs



"1" bit

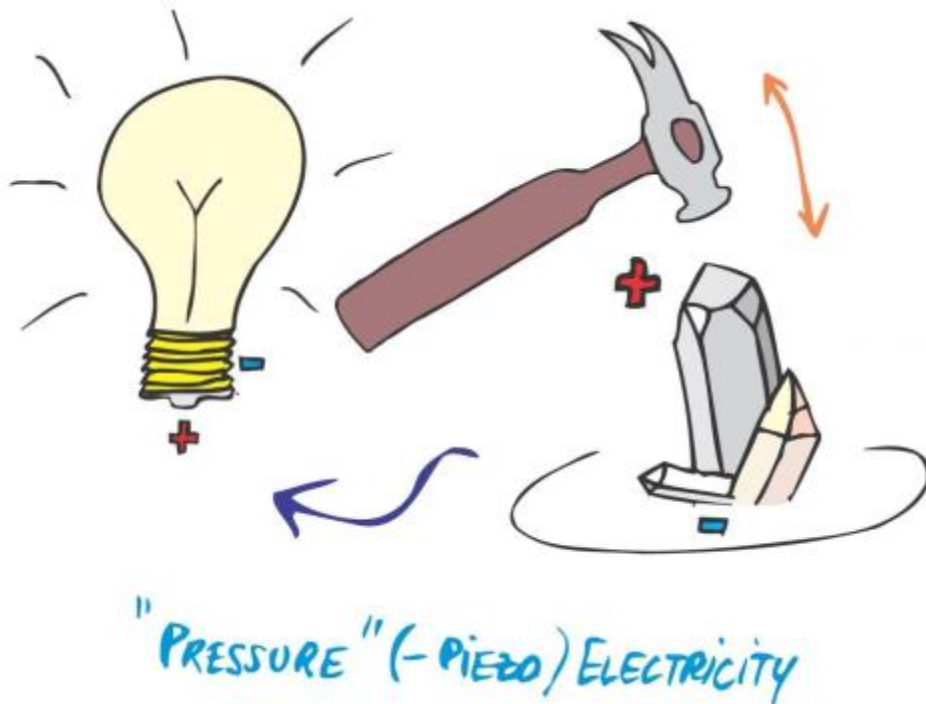
"0" bit



You will learn: MOF synthesis,
diverse characterization techniques,
strategies for control and design of MOFs

For more information contact Adrian Gonzalez (A.M.GonzalezNelson@tudelft.nl)

Piezoelectric Metal-Organic Frameworks for mechanical energy harvesting



What we want to know

- Which properties of MOFs affect their piezoelectric response? In which way?
- Is it possible to rationally tune a MOF for energy harvesting?

What you'll learn

- A broad variety of synthesis techniques
- Characterization of materials' structure and piezoelectric properties



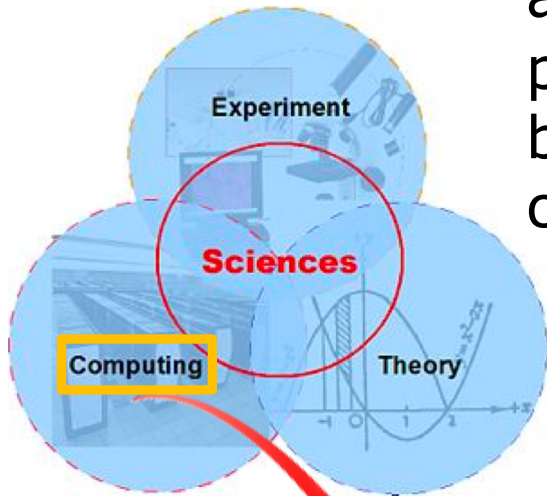
Contact:
Davide Rega
d.rega@tudelft.nl

MOFs: Flexible Piezoelectric Materials



Will Learn:

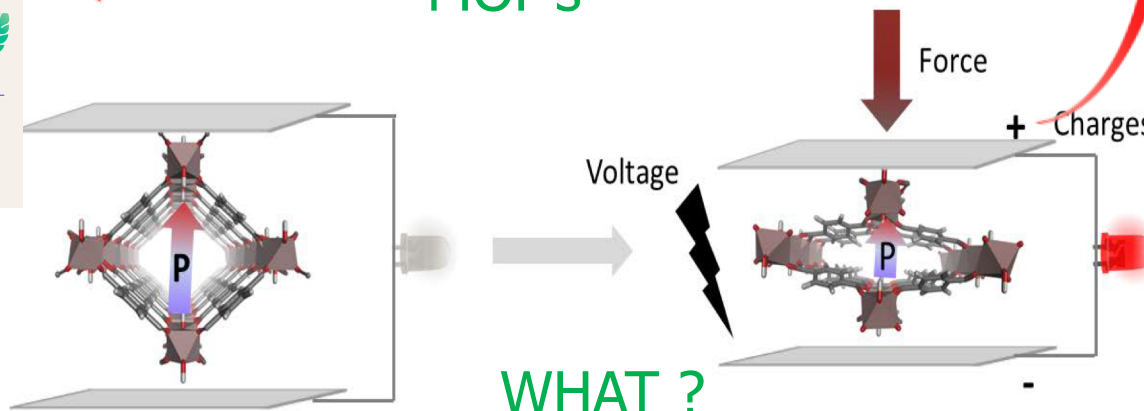
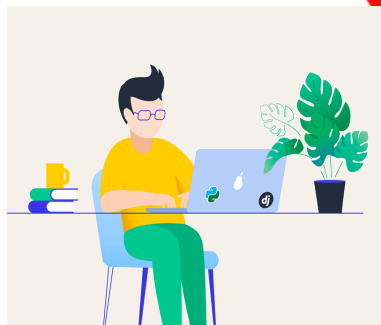
- a) to use CRYSTAL17 software to obtain piezoelectric properties
- b) Using Command line
- c) Basics of Quantum Chemistry



Computing Piezoelectric properties of a series of MOF's



HOW ?



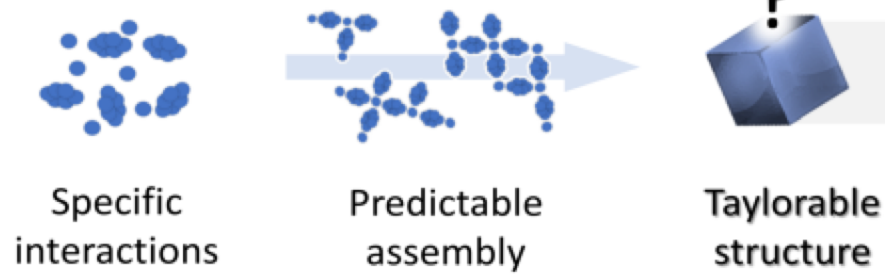
WHAT ?

For more information contact Srinidhi Mula (S.Mula@tudelft.nl)

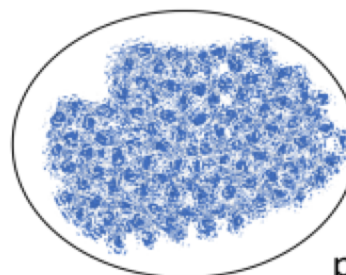
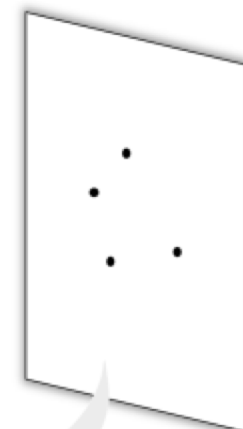
Growing bigger crystals for a deeper knowledge



Coordination polymers rational design



Single Crystal X-Ray Diffraction

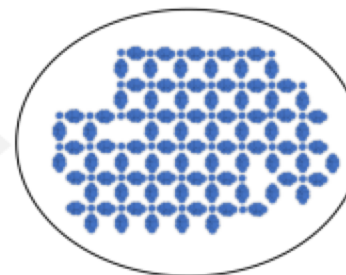
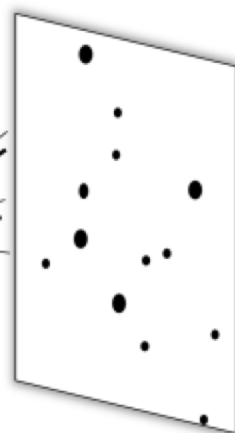
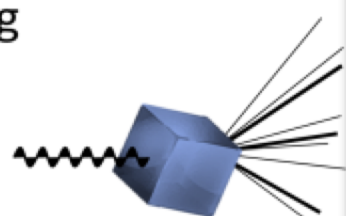


Poor resolution,
poor structural details

Synthetic conditions engineering



Large crystal
($>25 \mu\text{m}$)



Structure
determination with
atomic resolution

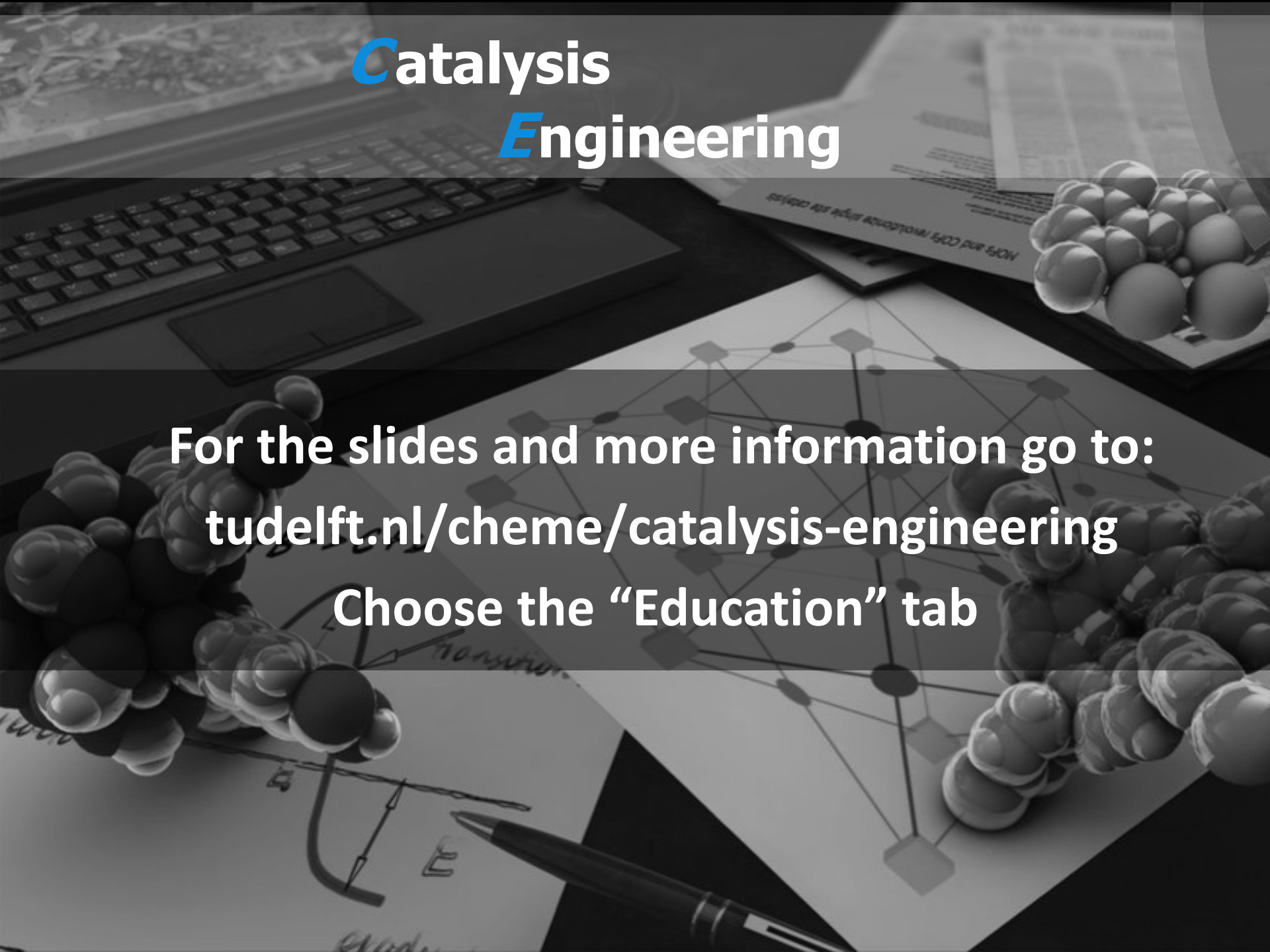
For more information contact Stefano Canossa (s.canossa@tudelft.nl)

Catalysis *Engineering*

After work: pizza, cake, BBQ, international dinner, Christmas dinner, cake, Friday drinks, and cake



Catalysis Engineering

The background is a grayscale collage of scientific and engineering-related images. It includes a laptop keyboard on the left, several sheets of paper with diagrams and text, and several 3D ball-and-stick molecular models of various structures. A network diagram with nodes and connecting lines is prominent in the center-right. A pen lies on a piece of paper in the bottom foreground.

For the slides and more information go to:
tudelft.nl/cheme/catalysis-engineering
Choose the “Education” tab