How can industry make use of the tools available at MAX IV & ESS
Workshop, 13 March 2017, Lund

The use of large research infrastructures in industrial catalysis

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HALDOR TOPSOE

Haldor Topsoe is a **world leader** in catalysis and surface science. We are committed to helping our customers achieve **optimal performance**.

We enable our customers to get the **most** out of their processes and products, using the **least** possible energy and resources, in the **most responsible** way.

This focus on our customers' performance, backed by our reputation for **reliability**, makes sure we add the **most value** to our customers and the world.

Haldor Topsoe
In brief

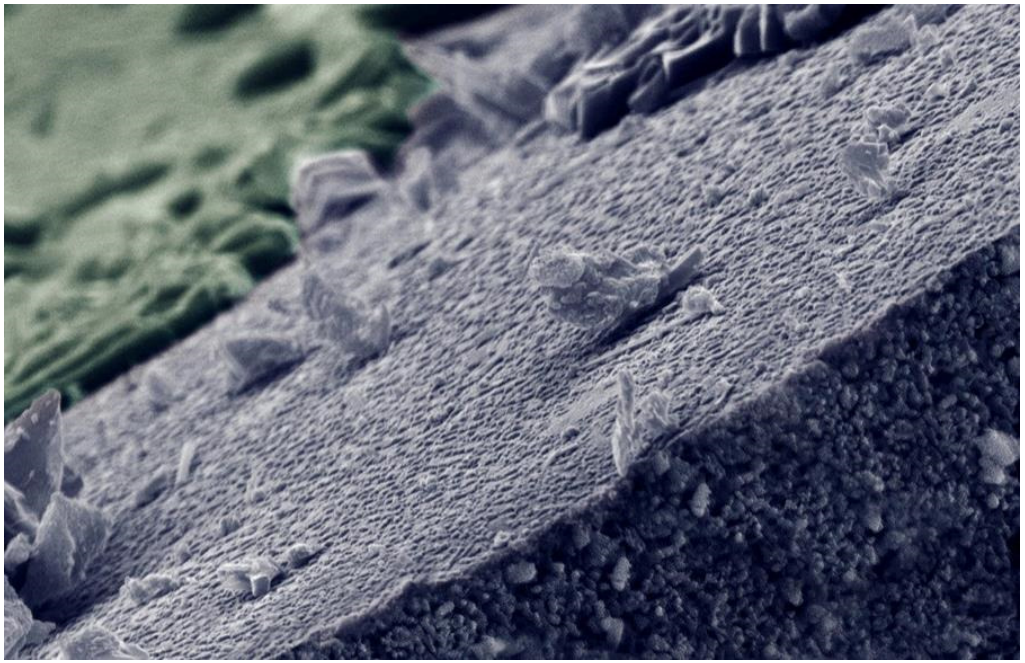
- Established in 1940 by Dr. Haldor Topsøe.
- Private 100% family-owned company.
- Market leader in heterogeneous catalysis and surface science for more than 75 years.
- 2,600 employees in 10 countries.
- Headquarters in Copenhagen, Denmark.
- Production in Frederikssund, Denmark, Houston, USA, and Tianjin, China.
- Spends around 10% of revenue on R&D.

2015 revenue
DKK 5,785M
(~ USD 850M)

2015 operating
profit DKK 502M
(~ USD 75M)

Catalysis and surface science have a vital role to play in tackling these challenges and realizing the opportunities

- Chemical processes are used in the production of countless everyday objects including food, fuel, electronics and medicine.
- Almost all chemical processes utilize catalysts, and more than 90% of all industrial products are made using catalysis in some way.
- In a catalytic process catalysts promote the chemical reaction without being consumed by the process themselves.
- When a catalyst catalyzes a chemical process, the chemical reaction happens faster, using much less energy while also avoiding the production of unwanted by products



Catalyst surface magnified to the micrometer scale in one of our electron microscopes

We provide a full range of products and services for a broad range of chemical processing, hydroprocessing and emissions management processes

Chemical Processing

Hydroprocessing

Emissions Management

Process design, engineering & licensing + High-performance catalysts + Proprietary equipment + Business & technical services

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Types of research infrastructure (RI) used by industry: What, how and why?

What:

- Type of industrial use of RI's:
  - mainly strategic R&D during product/process improvements
  - not basic research or quality control
  - Balance between techniques new for synchrotrons (fs methods, high brilliance nano-beams) and neutron sources and established techniques (high flux, robust techniques)

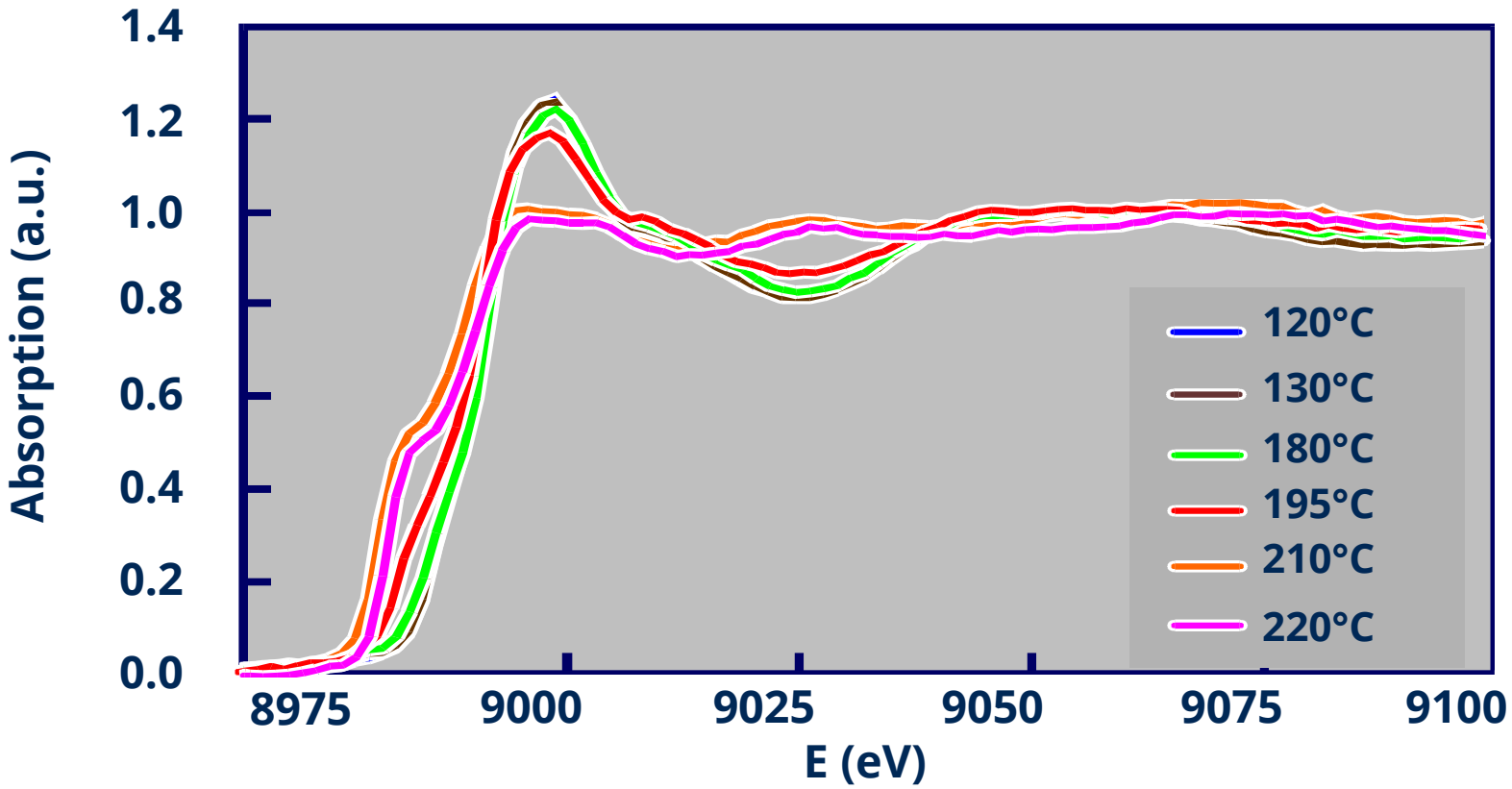
How:

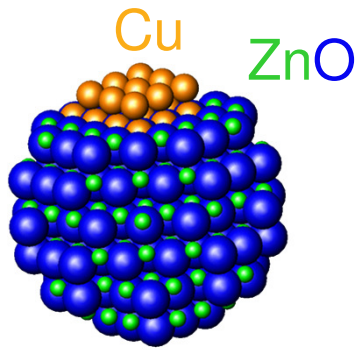
- Various ways to involve industry:
  - fully involved in experiments
  - collaboration with academic world e.g. via joint students, PhDs, Post-docs
  - analytical service (full analytical lab)
  - facilitation by mediator companies or industry portals, e.g. Colloidal Resource (SE), Finden Ltd (UK), Excelsus Structural solution SPRL (BE, USA), ScienceLink (Baltic Sea area), CINEMA (DK), SINE2020, LINX, …
- Often in close collaboration with academic groups

Why:

- X-ray (and neutron)-based techniques have nice properties to study catalysts under industrial relevant conditions: help improve our products and processes
- Scientific profile: relevant for e.g. customers, universities, employees

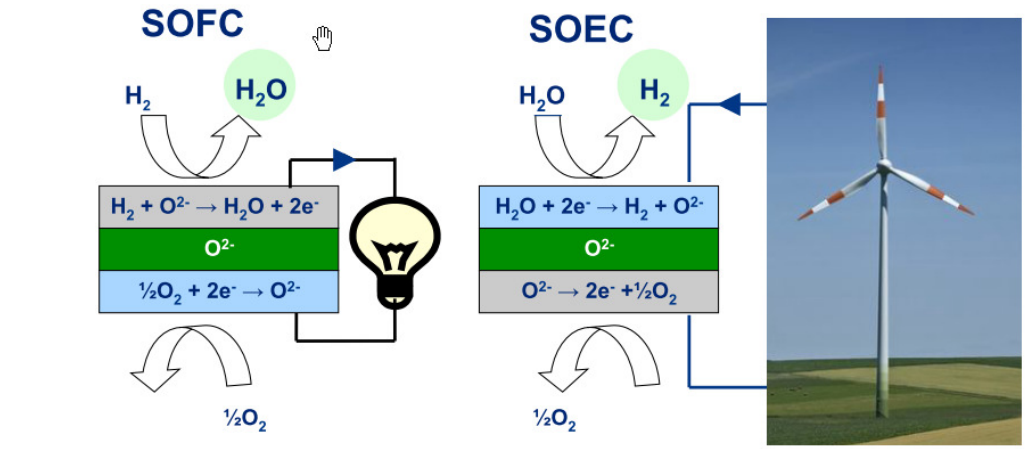
Activation of Methanol catalyst (Cu/ZnO) by Reduction - In Situ XAFS





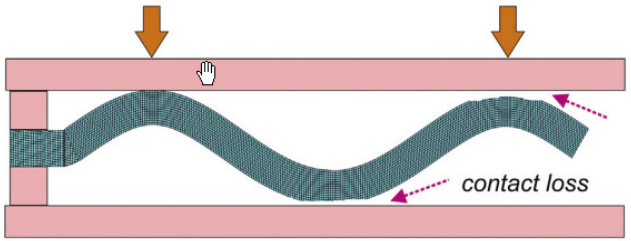
- Active site under reaction conditions: Cu
- Change of shape of Cu particles dependent on reduction potential: optimal load of reactor

Use of neutrons to improve SOEC for hydrogen production



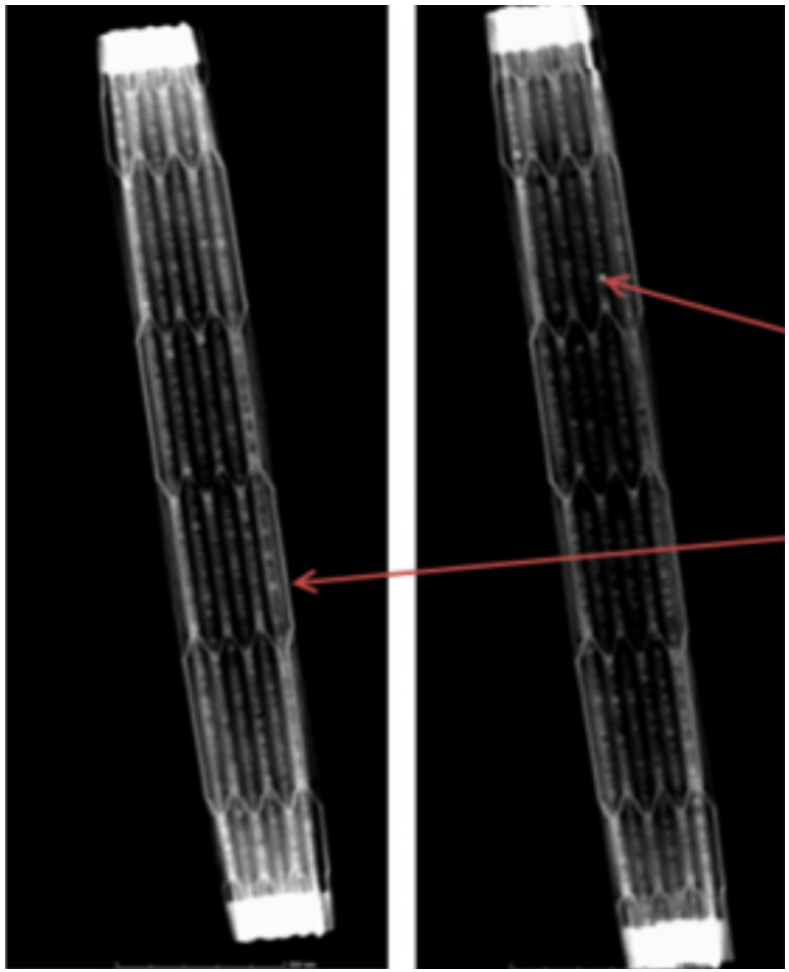
$$H_2 + CO + O_2 \underset{\text{SOEC}}{\overset{\text{SOFC}}{\rightleftharpoons}} H_2O + CO_2 + \text{electric energy } (\Delta G) + \text{heat } (T\Delta S)$$

- Electricity of renewable sources can be used by SOECs to produce H_2.
- During operation, some contacts between cell and interconnects are lost and extend and nature is unknown.
- Use neutron tomography to quantify differences between a fresh stack and a stack with known contact issues



T. Molla et al., *Int. J. Hydrogen Energy*, 41 (2016) 6433

Use of neutrons to improve SOEC for hydrogen production



- Neutron radiography (ANTARES) was used to image cells (centimeters of metal) in a non-destructive way
- Inhomogeneities were identified within the cells

Thanks to SINE2020, Maier-Leibnitz Center (TUM)

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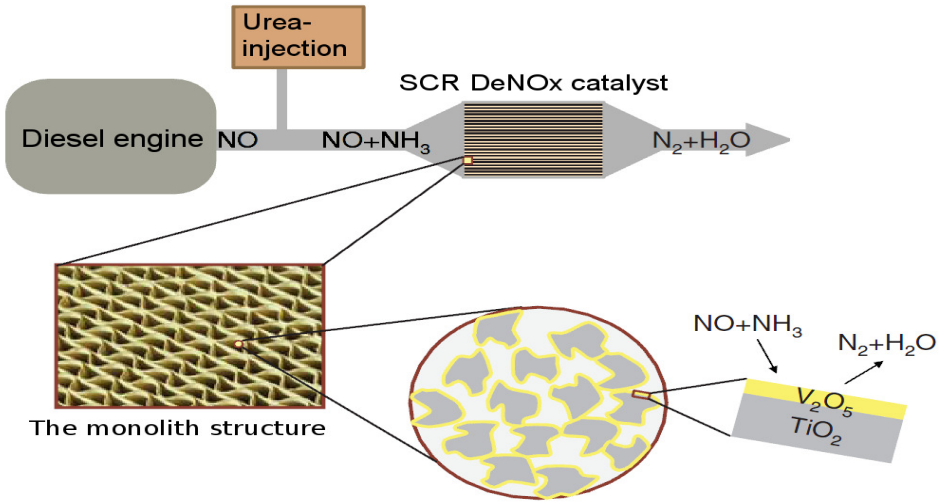
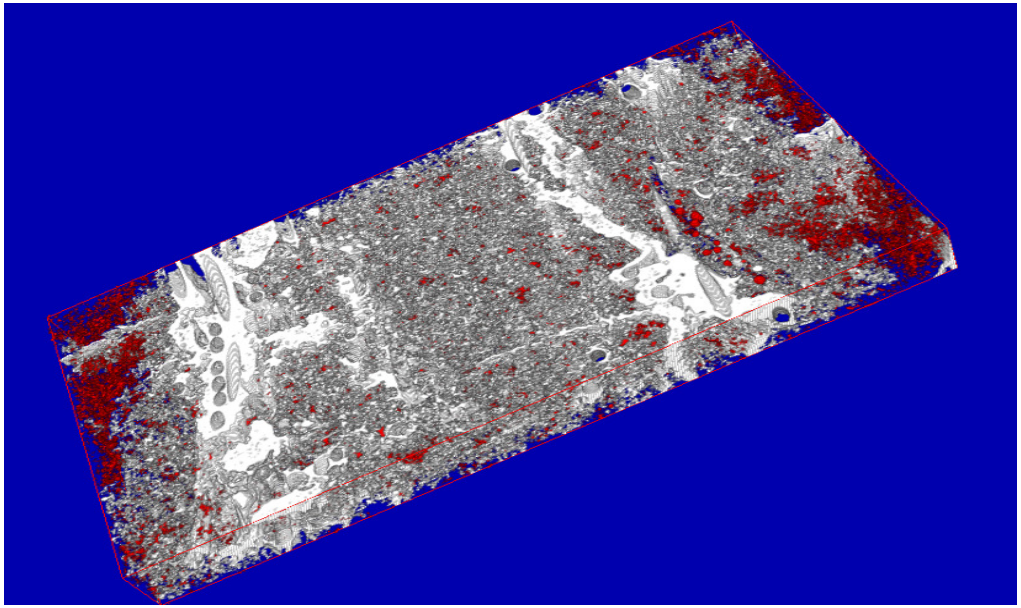
Pore system characterization in monolites for DeNOx applications





$4NO + 4NH_3 + 3O_2 \rightarrow 4N_2 + 6H_2O$

$2NO_2 + 4NH_3 + 3O_2 \rightarrow 3N_2 + 6H_2O$

$NO + NO_2 + 2NH_3 \rightarrow 2N_2 + 3H_2O$

- 350 nm resolution
- Closed porosity in red: 16% - way to improve activity
- Higher brilliance sources will improve usability, e.g. 3D mapping of chemical state/composition on 10-50 nm scale

Tomcat beamline, SLS, Villigen

Value of use of large infrastructure

- General improvement of understanding of catalysis and catalysts
- Improved understanding of our products and processes might lead to better products
- Our customers know that we continuously improve and help

What is needed?

- Passion for science, supported by company management and company owners
- Long-term, dedicated effort with competent staff
- Realistic view on results to be obtained
- Only a small part of our scientific effort, backed up by large in-house R&D activity
- Robust experimental techniques including state-of-the-art data analysis

Key challenges for industrial use of RI's

- Large cost/benefit ratio:
  - high expenses, large distance, travel costs, hotel, beam time/instrument time, equipment
  - many experienced researchers needed for one experiment
  - complex experiments, unique results?, complex data analysis
- Beamline/experimental staff:
  - lack of staff: experiments run 24 hours/day, but staff not always available
  - lack of experienced staff (short-term contracts)
- Full remote control of experiments is hardly possible
- Extra facilities, e.g. preparation labs, not always available
- Data deluge:
  - Lack of automated on-line data analysis and reduction software
  - Archiving / transportation of large data sets is a challenge
- Lack of standardization / certification / ISO standards and quality control:
  - Interfaces between beamline and sample environment
  - Data formats, standard protocols

Differences in goals and use between industry and academies/RI's

Industry:

- products + process + services

- larger amount of samples
- real catalysts
- peer review system for beamtime applications: not judged on technological quality or industrial relevance
- faster results are demanded: robust methods + on-line analysis
- fast access to facilities: reduced time from R&D to market
- focus on confidentiality, IPR, secrecy agreements resulting in bureaucracy

Academies / RI's:

- publications + fundamental understanding andbeamline and instrument oriented
- small amount of samples
- model catalysts
- peer review system for beamtime applications: judged on scientific quality

- RI's: more focused on unique methods

- Typical access after half a year

Limited interest in industrial use by many RI's

Thank You