syngaschem BV
synthesis gas chemistry
fundamental research projects

# Syngaschem BV
# Annual Report 2017

March 2018

SynCat @ Beijing
The Synfuels China Laboratory for Fundamental Catalysis
Science & Technology for Clean Fuels from Coal

SYNFUELS CHINA

*Syngaschem BV is Research Partner of SynCat@Beijing*

*and receives its base funding from*

*Synfuels China Technologiy Co., Ltd, Beijing-Huairou.*

syngaschem BV
synthesis gas chemistry
fundamental research projects

# Syngaschem BV
# Annual Report 2017

March 2018

## Highlights

- Research within two programs, namely the CHIPP project together with DIFFER Institute and the TU/e, co-funded by NWO and Syngaschem BV with base funding from Synfuels China, and in the CritCat Consortium with 9 European partners, funded by the EU-H2020 program.
- Publication of 10 papers on Syngaschem-based research, and 7 more together with SynCat@Beijing.
- Syngaschem staff gave 12 oral presentations at international conferences and universities in the USA, South Africa, China, Norway, Austria, and participated in three PhD defences in Norway, Denmark and Eindhoven.
- The book Concepts in Modern Catalysis and Kinetics by Ib Chorkendorff and Hans Niemantsverdriet reappeared in updated and extended version with Wiley-VCH (Weinheim) in August 2017
- The book Scientific Leadership by Jan Karel Felderhof and Hans Niemantsverdriet appeared with DeGruyter (Berlin) in December 2017.

SYNFUELS CHINA

SynCat @ Beijing
The Synfuels China Laboratory for Fundamental Catalysis
Science & Technology for Clean Fuels from Coal

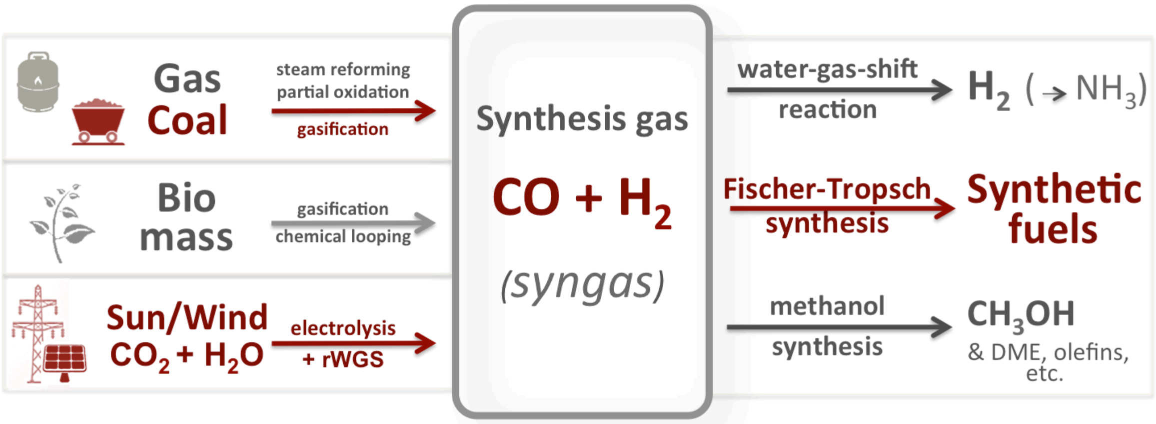
*Syngaschem BV is Research Partner of SynCat@Beijing and receives its base funding from Synfuels China Technologiy Co., Ltd, Beijing-Huairou.*

# Introduction: What is Syngaschem BV?

Syngaschem BV is a Dutch private research enterprise founded as research partner of Synfuels China Technology in China. Together they established a laboratory for fundamental research, entitled SynCat@Beijing. In fact, Syngaschem was started in 2013 to take care of recruitment of staff and planning of research program and infrastructure, in close collaboration with the executive leadership of Synfuels China. In addition, Syngaschem serves as the Dutch branch of SynCat@Beijing, with its own research program, under the name SynCat@DIFFER, and located at the Dutch Institute for Fundamental Energy Research at Eindhoven.

# Vision and Mission

The SynCat laboratories operate on the basis of the vision that synthesis gas ($CO + H_2$) is and will continue to be a crucial intermediate in clean energy technologies for the future, in many parts of the world. Synthesis gas can be obtained from traditional fossil sources, as well as from biomass and from electricity in combination with water and sources of carbon dioxide, see the scheme below. With the advent of renewable electricity from wind and solar energy, which is inherently intermittent, synthesis gas is the intermediate to high-energy density fuels that serve to store energy. In the context of Coal-to-Liquids Technology in China, such renewable sources of electricity can be applied to decompose water in hydrogen, to supplement the syngas, and oxygen to be used in the gasification step. In this manner, renewable electricity has the potential to significantly reduce the by-production of $CO_2$ that presently accompanies the use of coal.



The mission of Syngaschem BV is to obtain fundamental understanding behind the production of synthesis gas by renewable energy and its utilization to produce synthetic fuels for the storage of energy. It therefore concentrates on electrochemistry for water and $CO_2$ electrolysis, surface science and spectroscopy for understanding of CO hydrogenation reactions, both in combination with molecular modeling.

# The Year 2017 at a glance

After moving to the new DIFFER building in December 2015, Syngaschem started to build up its new laboratory there from January 2016 onwards. As some of the building infrastructure of the DIFFER institute was not ready, only part of the Syngaschem lab, predominantly the electrochemistry instrumentation, could be built up and used. After making the designs of the laboratory infrastructure to suit the research needs of Syngaschem BV the lab became available for installation of all equipment in the beginning of 2017. With the equipment being available experiments were performed until June 2017. On June 22, a small water cooling unit caught fire during the night which resulted in serious soot contamination of the laboratory. Consequently, all equipment had to be moved out and cleaned, causing a significant delay in the research. Fortunately, it was possible to find a temporary location elsewhere in the DIFFER institute so that experiments could be resumed in August 2017. We are greatly indebted to the management and the staff of the DIFFER Institute for offering help, among others, by allowing us to place setups in various laboratories of the Institute, so that research could go on.

Figure 1 A look into Syngaschem's office (left) and laboratory (right)

## Collaboration and interaction with SynCat@Beijing

Syngaschem BV is research partner of Synfuels China Technology Co. Ltd in Beijing – Huairou, and SynCat@DIFFER is the partner laboratory of SynCat@Beijing. Frequent interaction exists between the two laboratories, and several joint publications appeared, in the area of mechanistic Fischer-Tropsch research, and on electrolysis of water. The following list illustrates the frequent mutual contacts:

- Hans Niemantsverdriet made 5 visits to SynCat@Beijing in 2017, until illness prevented him to travel during the last Quarter of the year. Weekly plan and progress mails of all SynCat staff keep him up to date, while he is not at Beijing.
- Kees-Jan Weststrate visited SynCat@Beijing two times for a week, mainly for interaction with the surface science group. They also maintain regular contact by email on practical UHV and instrumental issues.
- Professors Jian XU and Xiaodong WEN visited Syngaschem BV between December 19 – 22. They were introduced to the ongoing research at Eindhoven, and had a progress meeting with Hans Niemantsverdriet, Kees-Jan Weststrate, and Jose Gracia, to discuss the way forward in 2018.

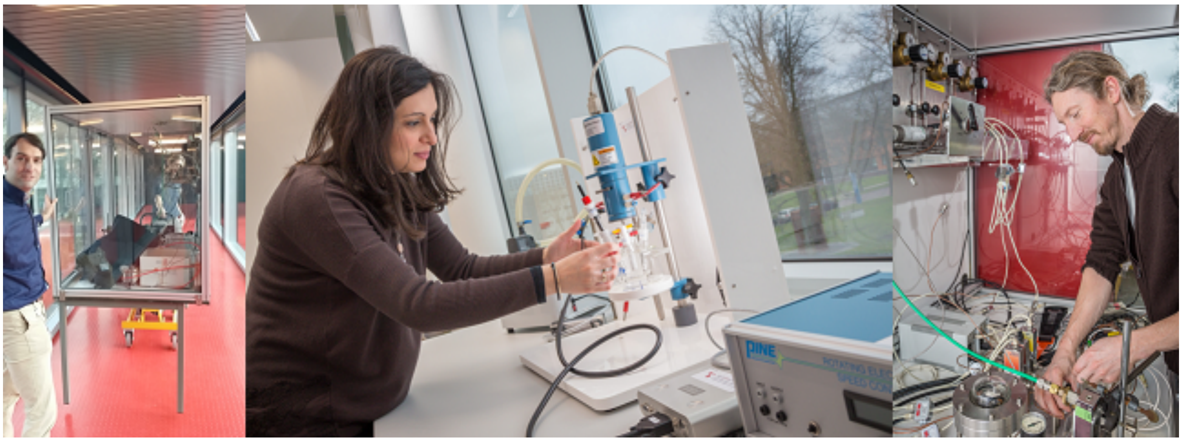


**Figure 2 Syngaschem staff at work in the laboratories at DIFFER:
Kees-Jan Weststrate (left), Foteini Sapountzi (middle) and Hans Fredriksson (right).**

## Syngaschem Staff and students in 2017

| Name | Major Activities | Special tasks |
|---|---|---|
| Dr Hans Fredriksson | In situ spectroscopy and micro reactor technology; $CO_2$ chemistry | EU - CritCat project |
| Dr Foteini Sapountzi (0.8 fte) | Electrochemistry; electrolysis | EU - CritCat project |
| Dr Kees-Jan Weststrate | Surface Science; Fischer-Tropsch Chemistry | SynCat@DIFFER research program |
| Mr Antonio Vaccaro (0.1 fte) | Office Manager | |
| Ir Jan Karel Felderhof (0.1 fte) | Director Strategy, Organisation and HR Development; SynCat Ac@demy | |
| Prof dr Hans Niemantsverdriet (0.6 fte) | Director Syngaschem BV | |
| **Students and funding programme** | | |
| Ms Devyani Sharma (NWO) | PhD student, SynCat@DIFFER research programme | |
| Mr Daniel Garcia Rodriguez (NWO) | PhD student, SynCat@DIFFER research programme | |
| Mr Marc Bonte (Fontys Univ of Applied Sciences) | MSc student; EU-CritCat project | |
| Ms Joana Zhou (Fontys University of Applied Sciences) | MSc student; EU-CritCat project | |

# Overview of Funding Sources

- Base funding from Synfuels China Technology Co. Ltd.
- NWO CHIPP Subsidy for research program together with the DIFFER Institute and TU/e
- European Union Horizon 2020 funding for the CritCat program
- Annual subsidy on labour costs in the form of tax deductions from the Ministry of Economic Affairs (WBSO)

Syngaschem BV has been established together with and based on funds provided by Synfuels China Technology Co. Ltd, with the mission to support the building up of SynCat@Beijing, which is our first and topmost priority. The long-term perspective offered by this partnership implies that Syngaschem can afford to invest in a laboratory with a durable research agenda, without having to resort to a strategy aimed at quick wins and short-term successes. The five-year period agreed with DIFFER for building up complementary activities of mutual interest for both SynCat@Beijing and DIFFER's solar fuel program fits well in this philosophy. In the meantime, Syngaschem sees it as its obligation to expand the possibilities for research by creating opportunities for PhD students and young postdocs to participate in the work, to create more impact and critical mass. After a highly successful year in 2016 with both the EU H2020 Grant for the CritCat project (3 year) and the NWO-CHIPP Program SynCat@DIFFER (5 year) awarded, the activities in 2017 were dedicated to looking into future funding possibilities after the completion of the CritCat project. To this end, Syngaschem BV participated in two new H2020 proposals described below.

### Annual Subsidy for Research Granted from the Dutch Knowledge Economy

Since April 2015, the Dutch Ministry of Economic Affairs acknowledges Syngaschem's research activities along our European strategy as a valuable contribution to the Dutch Knowledge Economy by granting a subsidy in proportion to the time spent on certain eligible research activities (nationally known as WBSO subsidy). The subsidy varies per year, but amounts to about 42.000 Euro in 2015, 75.000 Euro in 2016 and an estimated 85.000 Euro in 2017. Though these amounts may seem modest, they enable Syngaschem to engage in highly beneficial research collaborations with two universities in South Africa (Capetown and the Free State), for which additional funding would be difficult to acquire.

### Two New EU H2020 Project proposals submitted

In 2017, Syngaschem BV was invited to join in two European Consortia under the roof of the Horizon 2020 program. The first, TREEHOMES, aims at developing technology for electricity-to-gas, in small scale with the intermittent power supply typically generated by renewable source and the second, SAMM, aims at developing single atom catalysts for methane conversion to methanol.

Applications for the first part in a two-stage procedure have been prepared and submitted. Syngaschems share of the total budget of 5 -7 million euro over four years as requested would be on the order of 600.000 euro. If granted, these resources will be dedicated to research on electrocatalytic reactions, heterogeneous catalysis synthesis and testing and micro reactor developments. In case of success, Dr Sapountzi will lead Syngaschem's activities in electrochemistry while Dr Fredriksson takes care of heterogeneous catalyst testing. The expected start date for both projects in case of approval will fall in 2019.

# Research Program of Syngaschem BV

As a result of the generous base funding by Synfuels China, and the additional subsidies acquired in 2016, the research program for the coming years will consist of three major subjects:

1) **Fischer-Tropsch Chemistry,** led by Dr. Kees-Jan Weststrate, in collaboration with SynCat@Beijing, and with the DIFFER institute. Emphasis of the work is on understanding the mechanism, in particular in relation to selectivity patterns. An external collaboration with the University of Capetown focuses on the selectivity of FTS Catalysts for special products, and it has been running successfully in 2017. We will continue to fund these projects in 2018 as well.

2) **Electrolysis of Water and $CO_2$** led by dr Foteini Sapountzi, with support by Dr Hans Fredriksson. This program is carried out in collaboration with Syncat@Beijing on perovskites for the oxygen evolution reaction, and on alcohol reforming for hydrogen production. Within the CritCat consortium the emphasis is on testing novel formulations based on computational predictions for $H_2$ evolution. In a collaboration with the University of the Free

State in South Africa, we will study cluster derived iridium-ruthenium systems for the oxygen evolution reaction.

3) **Model Catalysts and Micro Reactors for in situ studies** led by dr Hans Fredriksson. Focus of the work has been to study Cu-based catalysts for $CO_2$ activation with optical plasmon resonance techniques inside microreactors. In the framework of the CritCat Project, catalysts will be tested for $H_2$ formation by ammonia decomposition. Though the collaboration that was established with Dr Peter Thüne at Fontys University of Applied Sciences a successful bachelor student project was performed under Hans' supervision. In this project catalysts, in part prepared by our partners at UCT, Cape Town, were tested for the ammonia decomposition reaction.

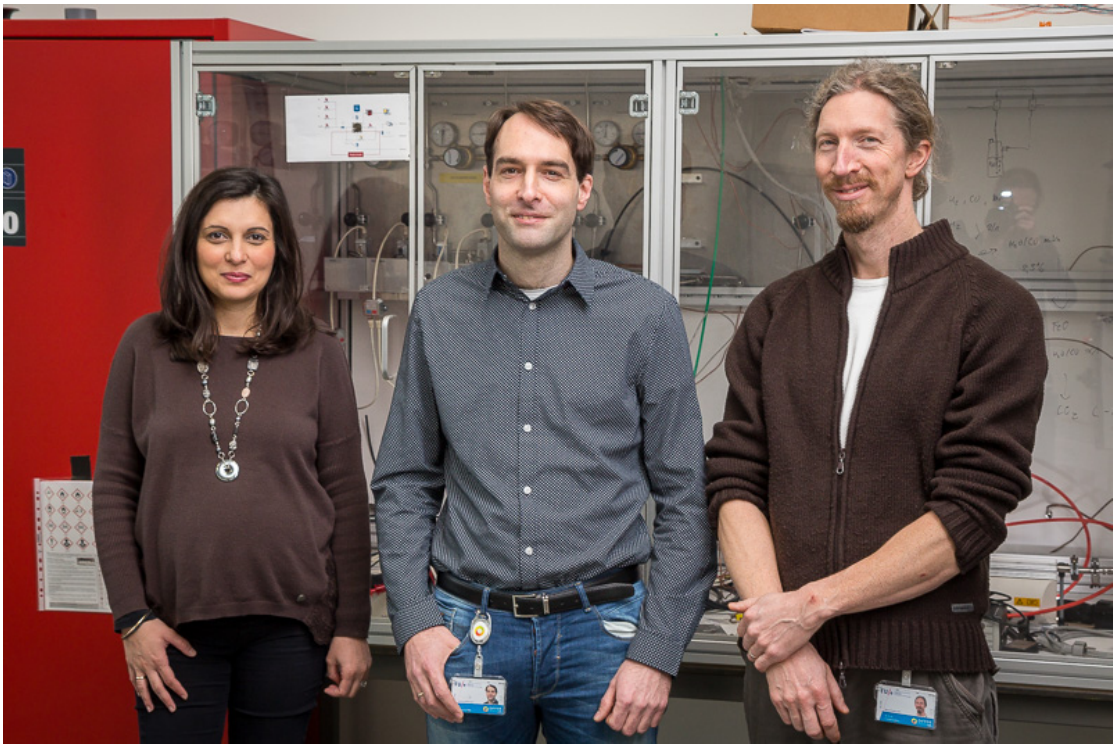


**Figure 3. From left to right: Dr Foteini Sapountzi, Dr Kees-Jan Weststrate, Dr Hans Fredriksson**

## Research Highlights 2017

### 1) Fundamentals of the Fischer-Tropsch reaction (Dr. Kees-Jan Weststrate)

Two projects are performed in the Syngaschem Laboratories in the context of the SynCat@DIFFER programme. Project 1 focuses on understanding the influence of surface structure of various elementary reaction steps on the surface of cobalt catalysts. In 2017 this project was kicked off by an investigation of the adsorption of CO and $H_2$, reactants in the FTS reaction.

The adsorption of both CO and hydrogen is being studied using three different single crystal surfaces of cobalt, shown in figure 4(b). The Co(0001) sample exposes large close-packed terraces and serves as a reference as it has been studied extensively before. The Co(11-29) sample exposes step edges which, in the bulk-terminated structure, exposes a step edge consisting of 6 and 8-coordinated atoms, so-called kink sites. Next to the atoms at the step edge the close-packed terrace consists of only three atomic rows, a relatively narrow terrace. The (1 0 -1 20) surface exposes 9-atom wide close-packed terraces separated by mono-atomic steps consisting which consist of atoms with a coordination number of 7. Due to the hcp structure of the cobalt single crystal the step geometry alternates between the B5-A and B5-B type.

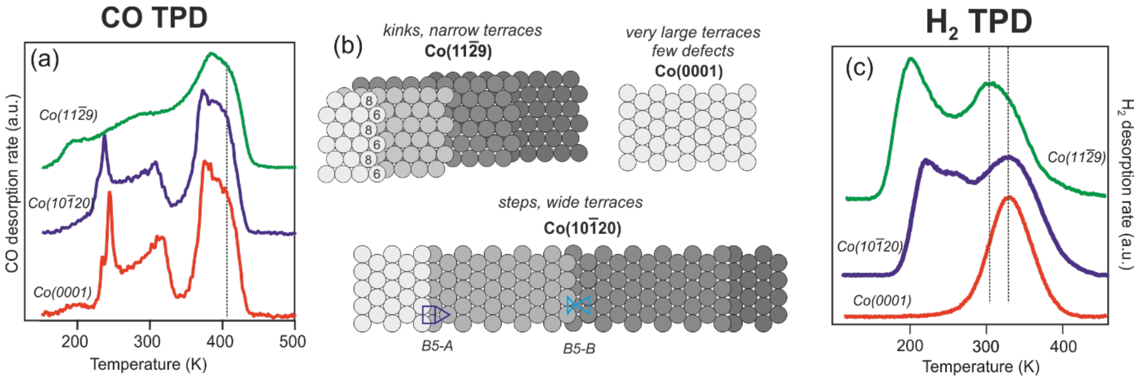


**Figure 4: (a) CO and (c) $H_2$ desorption spectra after saturating the Co surface at 100 K with either CO or $H_2$. Three different surfaces of Co were compared, with the structure of each shown in (b).**

The desorption peak around 400 K found in the CO TPD spectra for these three surfaces, shown in figure 4(a), corresponds to desorption of the last bit of CO from the surface, and its desorption temperature can be taken as an indication of the adsorption energy of CO on the surface. The absence of a high temperature desorption peak in the spectra for the stepped surfaces indicates that CO does not adsorb more strongly on step and kink sites. The CO desorption peaks <320 K corresponds to the situation where the CO coverage is high. The two different desorption peaks around 320 K and 250 K on the flat surface are attributed to ordered adsorbate structures with a high CO density, i.e. for these peaks the adsorbate-adsorbate interaction plays an important role in the desorption temperature. The ordered structures that give rise to the desorption peaks at 300 and 250 K on the flat surface have a large unit cell, and they cannot be formed on the Co(11-29) surface because the close-packed terraces are only three atoms wide. Consequently, the desorption peaks associated with these structures become broader and shift to lower temperatures. Instead, the terraces on the Co(10-120) surface is very small: The 9-atom wide terraces are big enough so that the same ordered structures can form as in the case of Co(0001). A close inspection shows that the desorption peaks <320 K are shifted downward by ~10 K. This is taken as an indication of a slight destabilization of these ordered layers due to the finite size of the terraces compared to the flat surface.

On the flat surface dissociative adsorption of $H_2$ is not very efficient and is associated with a small sticking coefficient. Undercoordinated sites such as steps and kinks strongly enhance $H_2$ dissociation. Assisted by defects to dissociate $H_2$ the hydrogen coverage at the saturation point is found to be twice high as on the flat surface, where the hydrogen >0.5 ML desorbs below room temperature [see figure 4(c)].

These findings show that (i) the size of the terrace affects the CO adsorption behaviour, and (ii) step and kink sites are not only essential for (direct) CO dissociation but they also play an important role in the supply of $H_{ad}$ to the surface under FTS conditions. The surface hydrogen concentration (as well as the vacant sites available for H to adsorb) appears in practically all kinetic equations describing the elementary reaction steps required to produce a long hydrocarbon chain starting from CO and $H_{ad}$. This implies that both FTS activity and selectivity are strongly influenced by the surface structure of the active catalyst surface.

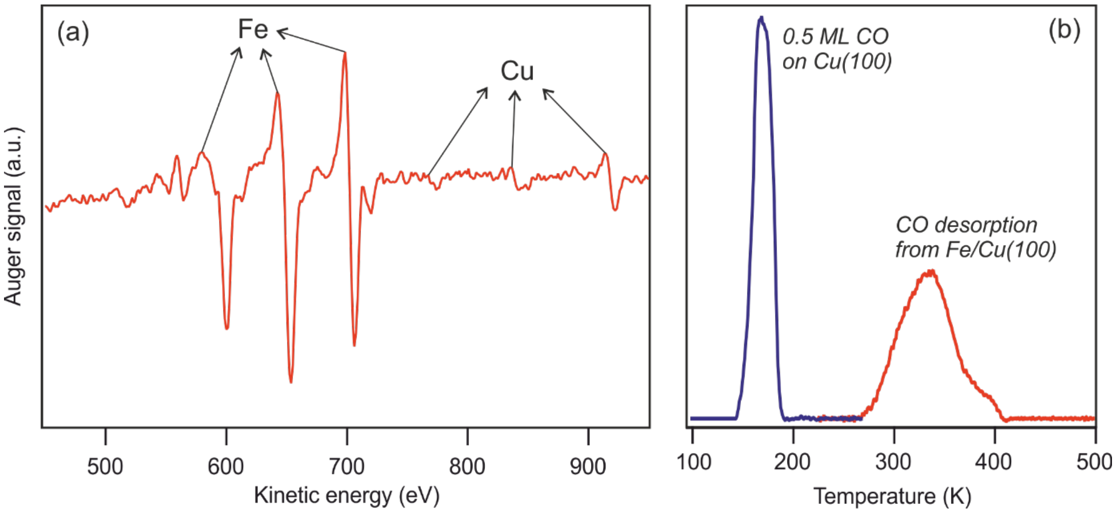


**Figure 5: (a) Auger electron spectrum after Fe evaporation onto a Cu(100) substrate. (b) CO TPD before and after Fe evaporation**

The second project aims to prepare iron carbide model catalysts by evaporation of iron into a copper substrate followed by treatments to carburize the sample. After installing the iron evaporator in mid-December several exploratory experiments were performed. Figure 2(a) shows the Auger electron spectrum recorded after evaporating iron. The large signal of Fe, combined with the small Cu signal indicates that the evaporated layer consists of around 10-20 ML of Fe. The CO TPD spectrum recorded afterwards [fig. 2(b)] confirms this, as the desorption peaks due to CO bound to copper (150-200 K), have disappeared, and instead a CO desorption peak is found around 320 K, attributed to CO adsorbed on iron.

## 2 Electrocatalysis for storing renewable energy in chemical bonds (Dr Foteini Sapountzi)

- Hydrogen production through the electrochemical reforming of C1-C3 alcohols

Electrochemical reforming of alcohols (also known as alcohol electrolysis, or organic solution assisted water electrolysis) has emerged as an alternative and promising approach for $H_2$ production using polymeric electrolytes. The power demands of this process are significantly lower compared to water electrolysis, thus this technology can offer remarkably reduced costs during long-term operation.

A research article dealing with hydrogen production through the electro-reforming of short-chain alcohols (methanol, ethanol, iso-propanol) and their mixtures using commercial gas diffusion electrodes and polymeric $H^+$ conductors, was published jointly with DIFFER and Synfuels China. We refer to the reference list at the end of this report. This study has been also presented as a poster in the 1st International Conference on Electrolysis.

For the continuation of this project, our aim in 2017 was to identify promising membrane-electrode-assemblies (MEAs) which can enable cost-effective and efficient alcohol electrolysis using methanol, ethanol and iso-propanol as the organic feedstock. For the purpose of this study, we worked jointly with DIFFER, Tu/e and BAS. Our investigations were focused on properly selecting both elements of a Membrane Electrode Assembly; i.e. the polymeric electrolyte and the gas-diffusion electrodes.

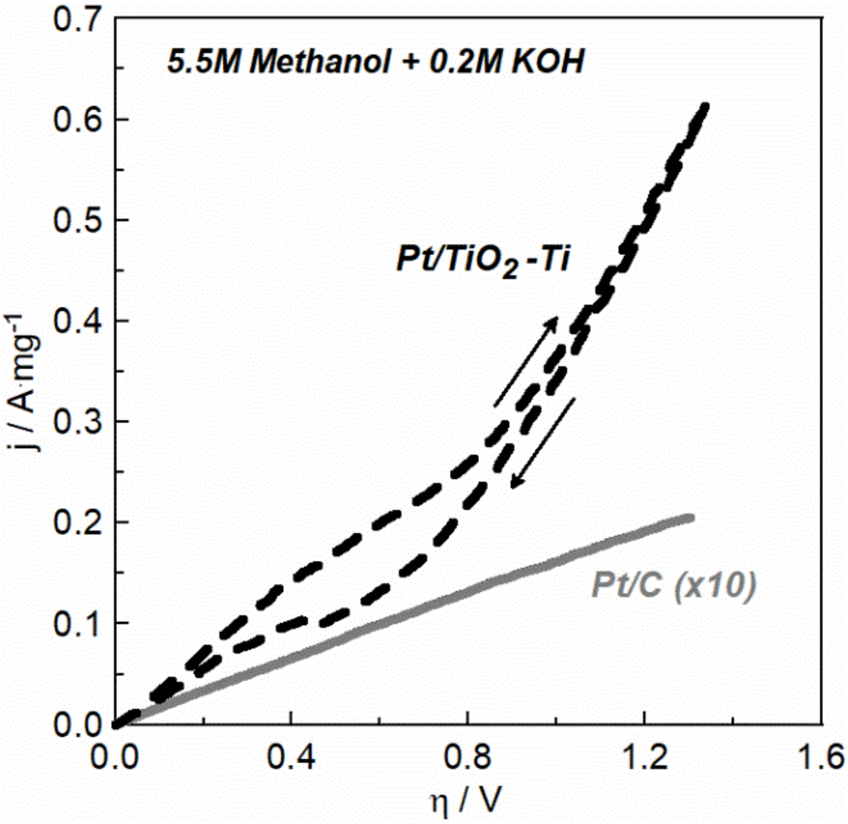


**Figure 6: Polarization curves during methanol electrolysis using the novel Pt(ALD)/$TiO_2$-Ti electrode and the commercial Pt/C carbon cloth electrode interfaced to a polymeric membrane with $OH^-$ conductivity (KOH-doped PBI membrane). Anolyte: 5.5M $CH_3OH$+0.2M KOH. Sweep rate is 10 mV/s.**

Regarding the effect of the polymeric electrolyte, and thus the acidity/alkalinity of the anolyte solution, we investigated the electrolysis of alcohol-water solutions using $H^+$ and $OH^-$ conducting membranes. At the best of our knowledge, no comparison exists in literature between alcohol-water electrolysers operated with $H^+$ and $OH^-$ conducting membranes under identical conditions.

To address the issue of catalyst utilization, a new type of gas diffusion electrode was developed via the Atomic Layer Deposition (ALD) of Pt on a porous $TiO_2$-Ti substrate. For comparison reasons, identical experiments were carried out also using commercial Pt/C on carbon cloth electrodes.

Overall, our results suggest that alcohol electrolysis can be more efficient using $OH^-$ conducting membranes under appropriate operation conditions (high pH in anolyte solution). Moreover, it was found that the ALD technique can result in up to ~30 times higher catalyst utilization compared to commercial Pt on carbon cloth. Figure 3 shows the overall cell performance when using as the anode the novel Pt/$TiO_2$-Ti electrode and the commercial Pt/C electrode. To enable comparison, per-mass normalized currents are presented in the polarization curves, while j values are multiplied by 10 for the case of commercial Pt/C anode. Literature studies report 5-10 fold enhancement in the performance of PEM fuel cells and water electrolyzers upon depositing Pt with ALD on carbon gas diffusion electrodes, which is typically attributed to the uniform structural characteristics of Pt due to the deposition technique. The superior enhancement obtained here is also the result of the metal-support interactions between the nanosized Pt particles and the $TiO_2$-Ti substrate, which are known to affect the electrocatalytic oxidation of alcohols.

Based on these results, an article manuscript has been already drafted and is planned to be submitted for publication, while this work has been accepted as poster presentation in the NCCC XIX conference.

- Evaluation of electrocatalysts for PEM water electrolysis

In the framework of CritCat, rationally designed noble metal-free electrode materials are tested under industrially relevant conditions in a PEM electrolysis unit.

As a first step, industrial metal sulphides provided by Tribotecc GmbH were evaluated as hydrogen evolution electrocatalysts. PEM water electrolyzers were operated under electrolysis of water vapor at 60°C, while commercial $IrO_2$ electrocatalysts were used for the oxygen evolution reaction. Figure 7 shows the polarization data recorded using three different sulfide cathodes (left), while also a comparison with the performance of the Pt cathode is presented (right). FeSx is the less active cathode, while MoSx is the most active cathode in the tested potential range. Doping $FeS_x$ with Cu enhances its activity which presents the highest Tafel slope among the three sulfides, however its onset potential is still lower compared to $MoS_x$. The overall activity of the sulfides is much lower compared to that of the commercial Pt electrode. This significantly low performance can be (i) either due to the large particle sizes (SEM on the sulfide electrodes showed particles of μm size, while the Pt nanoparticles in the commercial Pt on carbon cloth electrode have an average diameter of <10nm), (ii) or due to impurities in the industrial catalysts (XPS and ICP characterization is in progress to identify and quantify impurities).

For the continuation of these activities, planned experiments include (a) ball milling of the sulphide powders in order to decrease particle size, (b) preparation of MoS2 by ALD or electrodeposition.

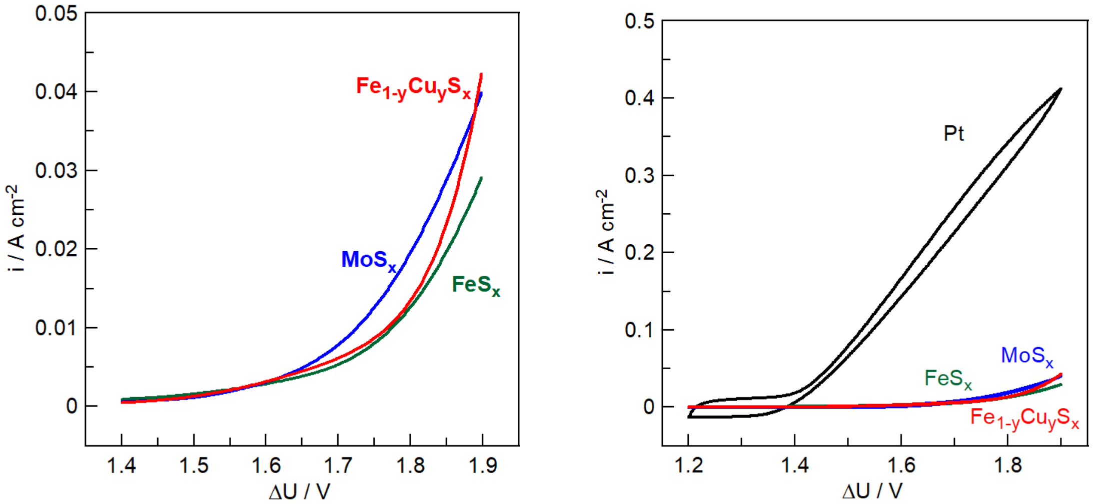


**Figure 7: Polarization curves during electrolysis of water vapor at 60°C. Left: Comparison of the performance using different metal sulfides as HER catalysts. Right: Comparison of the performance using metal sulfides and commercial Pt cathodes.**

- Electroreduction of $CO_2$ using polymeric electrolytes

In the framework of Critcat and in collaboration with DIFFER, the electrochemical fixation of $CO_2$ by $H_2O$ was studied in a novel reactor design. In essence, we used a reactor design of PEM electrolysis (gas diffusion electrodes and polymer electrolytes) for the simultaneous electrochemical reduction of $CO_2$ and oxidation of $H_2O$ to make syngas ($CO+H_2$) at room temperature.

While a configuration involving a $H^+$ conducting membrane (commercial Nafion) was shown to be unfavorable for $CO_2$ reduction, a modified configuration based on $OH^-$ conducting membrane (commercial Sustainion) allows for a great enhancement of the cathode selectivity for $CO_2$ reduction to CO. For addressing the material challenges, we have examined several cell configurations using the state-of-the-art $IrO_2$ as anode and Pt, Au and Ag as cathode. Detailed analysis of products and reactants allowed us to investigate in detail the three reactions which take place simultaneously at the cathode:

reaction 1: $3CO_2 + H_2O + 2e^- \rightarrow CO + 2HCO_3^-$
reaction 2: $2CO_2 + 2H_2O + 2e^- \rightarrow H_2 + 2HCO_3^-$
reaction 3: $2H_2O + 2e^- \rightarrow 2OH^- + H_2$

As shown in figure 8, hydrogen evolution is the predominant reaction on both Ag and Au, while the production rate of CO is one order of magnitude higher on Ag. This work has been accepted as poster presentation in the NCCC XIX conference and will be published in 2018.

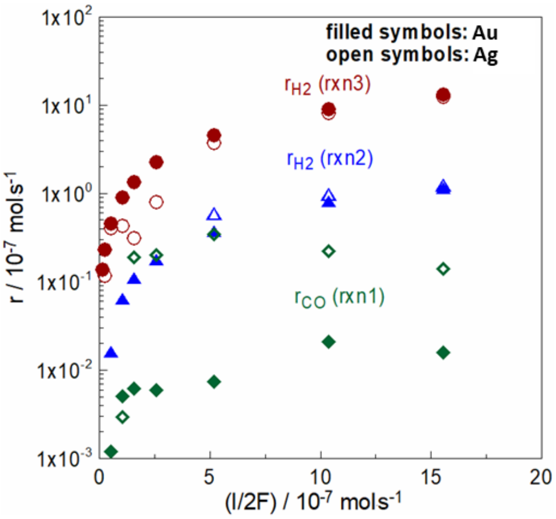


**Figure 8. Electro reduction of $CO_2$: Rates of reactions 1, 2 and 3 upon application of step currents. Ag cathodes appear an order of magnitude more active for $CO_2$ reduction than Au cathodes.**

## 3 Model catalysts and micro reactors for syngas related research (Dr Hans Fredriksson)

- Micro reactor and Cu-catalysts

Supported/promoted Cu catalyst are frequently used to synthesize methanol from syngas as well as for the low-temperature water-gas shift reaction (WGS). The in-house developed micro reactor with in-situ UV-vis spectroscopy has been further improved and used to monitor changes in the oxidation state of a $CeO_x$-promoted Cu catalyst as a response to changes in the feed gas composition.

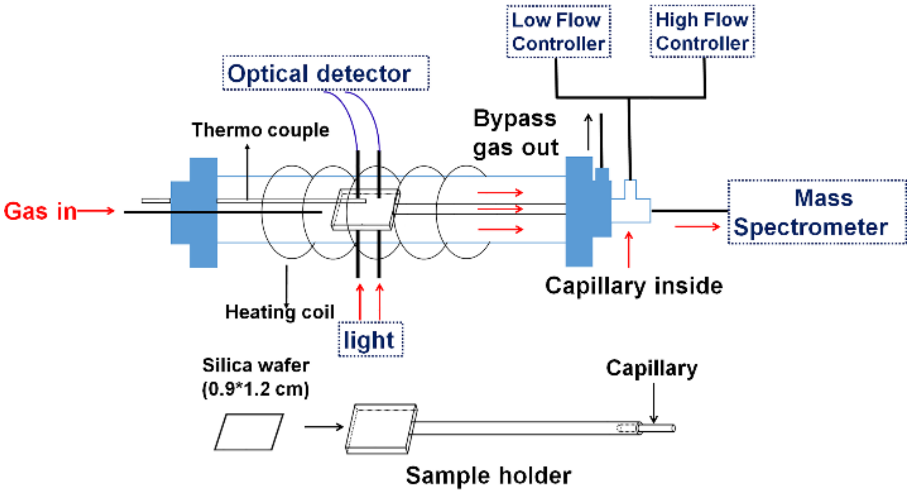


Figure 9: Micro reactor with in-situ UV-vis and mass spectroscopy for model catalyst testing

The results of testing flat model catalysts of Cu and Cu/$CeO_x$ under conditions relevant for selective oxidation of CO in $H_2$ have been written up in a paper published in Journal of Catalysis (DOI: 10.1016/j.jcat.2017.11.014). The work also includes computational input from a collaboration with DIFFER. The most notable findings are that the catalysts show excellent selectivity towards CO-oxidation. The catalysts activity is superior when Cu can be maintained in the metallic phase. However, metallic Cu is easily oxidized under process conditions.

- Model catalysts for FTS and $NH_3$ decomposition

Model catalysts consisting of size selected Fe and Fe/Mn nanoparticles on silica supports have been prepared and their activity tested under FTS conditions in a collaboration between TU/e, Sasol and Syngaschem. These results have been written up and published in Applied Catalysis A (DOI: 10.1016/j.apcata.2017.02.023). The most important results are that Mn improves stability of the Fe catalysts and alters the selectivity. Characterization also shows encapsulation of the active material in carbon layers, some sintering and catalyst reduction/$FeC_x$ formation during use.

The other set of model catalysts were prepared for the study of catalytic $NH_3$ decomposition, a reaction that is desired in the CritCat project. $NH_3$ acts as a poison for FTS catalysts but is also a valuable commodity for fertilizer production and it can be used as an energy carrier and a convenient way to store hydrogen. At present, Ru is the most efficient $NH_3$ decomposition catalyst, but the process is reasonably fast on a range of other materials, including Co and Fe. A range of alumina supported, monometallic, model catalysts were prepared and toughly tested. These measurements serve as a reference for future tests of bimetallic catalysts, where the aim is to replace Ru with cheaper materials while maintaining the high activity. The most important finding so far is that the activity of the Ru catalysts is greatly improved on size selected nanoclusters. Further experiments aiming at fabricating and testing bimetallic model catalysts and to elucidate $NH_3$ as a poison for FTS catalysts are being conducted.

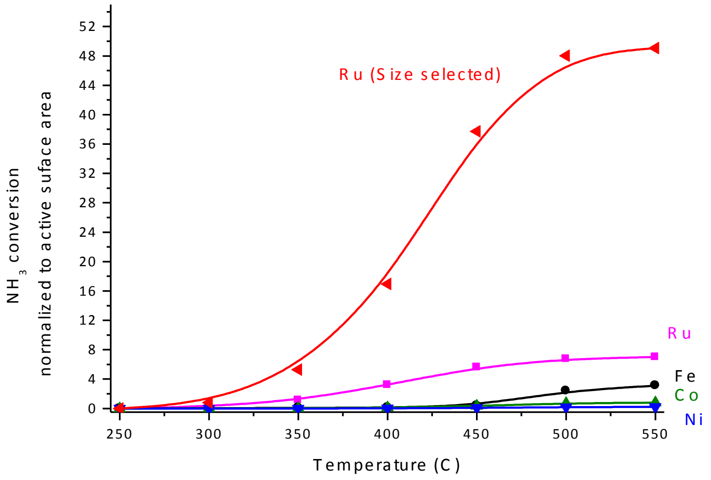


**Figure 10: $NH_3$ conversion as a function of temperature on a range of monometallic model catalysts**

- Catalytic combustion of volatile organic compounds (VOC)

VOC is present in exhaust from power plants and chemical factories as well as in solvents plastics and paints, contributing to air pollution, health problems and smog formation. It is thus desirable to eliminate the VOCs using catalytic combustion. Pt is a very efficient catalyst for this process but too expensive. Alternative catalysts have been prepared by flame spray pyrolysis and tested using toluene as a model VOC. It has been found that the catalyst support can play an important role in the catalyst efficiency. Ceria is even active without inclusion of Pt. These results are presently being written up for a publication. The research is conducted in collaboration with groups from Italy, Germany and Portugal within the framework of the CritCat project.

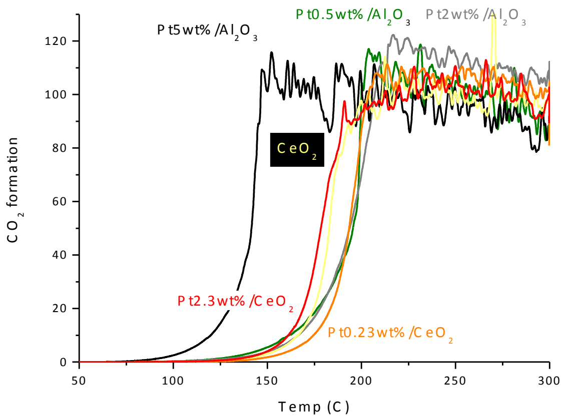
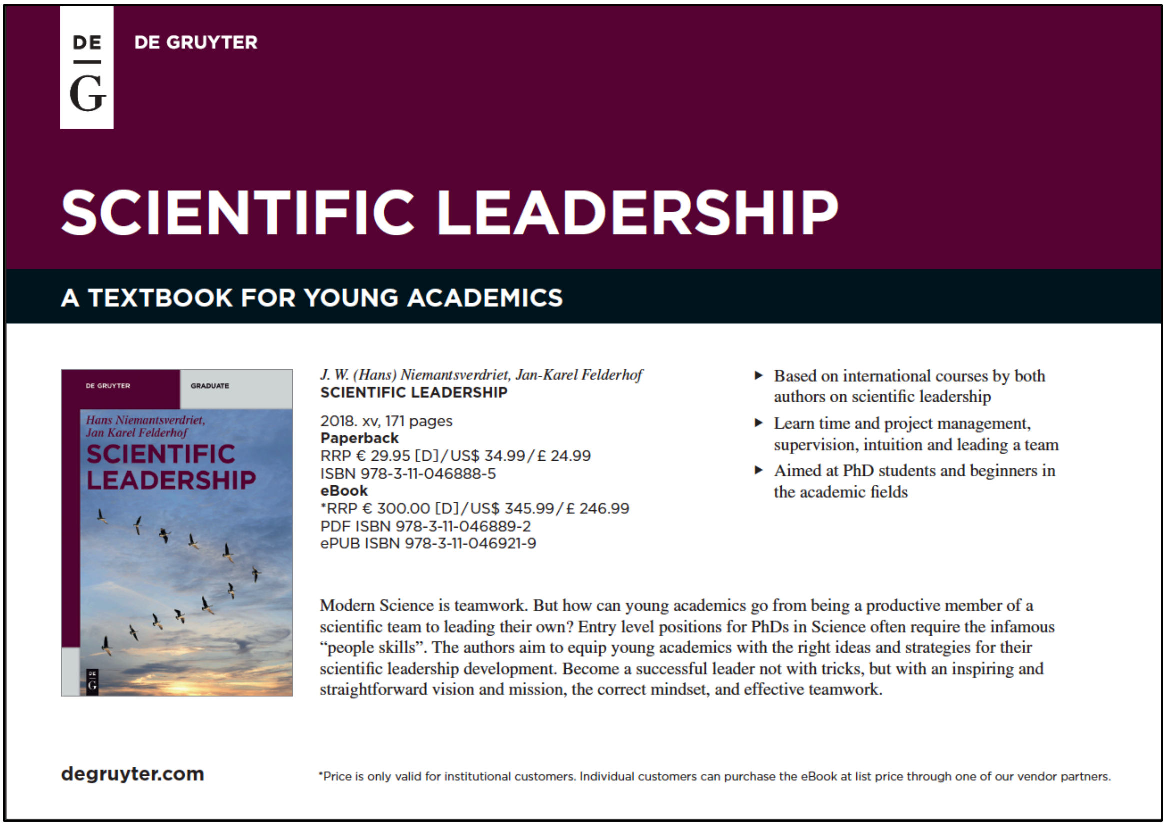


**Figure 11: $CO_2$ formation during catalytic combustion of VOC on Pt catalysts supported on $Al_2O_3$ and $CeO_2$**

## International Collaboration: Universities in South Africa

Under direction of Prof J.C. Swarts at the University of the Free State in Bloemfontein, South Africa, Drs Buitendach and Erasmus have performed very interesting research on the synthesis and characterization of Mn-Fe$_n$ multinuclear clusters, in a project that is sponsored by Syngaschem BV. Our interest is to use these elegant complexes as precursors for precision catalysts on the model scale. The work has so far led to publications on the synthesis in Inorchemic Chemistry, and on photoemission studies in Molecules, while a third publication on electrochemical properties is in progress. The work will be extended to the synthesis of Ir – Ru multinuclear clusters of similar structure, as well as porphyrine and phtalocyanide as candidates for electrocatalysts.

Syngaschem BV also sponsors collaborative projects in the Research Group of Prof Michael Claeys at the University of Capetown, on the subject of catalyst behavior in the Fischer-Tropsch reaction as studied by magnetic methods and X-ray diffraction, and on FTS product selectivity with a focus on specialty chemicals. These projects have started recently.



DE GRUYTER

# SCIENTIFIC LEADERSHIP

## A TEXTBOOK FOR YOUNG ACADEMICS

*J. W. (Hans) Niemantsverdriet, Jan-Karel Felderhof*
**SCIENTIFIC LEADERSHIP**

2018. xv, 171 pages
**Paperback**
RRP € 29.95 [D]/US$ 34.99/£ 24.99
ISBN 978-3-11-046888-5
**eBook**
*RRP € 300.00 [D]/US$ 345.99/£ 246.99
PDF ISBN 978-3-11-046889-2
ePUB ISBN 978-3-11-046921-9

- Based on international courses by both authors on scientific leadership
- Learn time and project management, supervision, intuition and leading a team
- Aimed at PhD students and beginners in the academic fields

Modern Science is teamwork. But how can young academics go from being a productive member of a scientific team to leading their own? Entry level positions for PhDs in Science often require the infamous “people skills”. The authors aim to equip young academics with the right ideas and strategies for their scientific leadership development. Become a successful leader not with tricks, but with an inspiring and straightforward vision and mission, the correct mindset, and effective teamwork.

degruyter.com

*Price is only valid for institutional customers. Individual customers can purchase the eBook at list price through one of our vendor partners.

**Figure 12: In December 2017 the book Scientific Leadership appeared, with a special foreword by Yong-Wang Li, and guest contributions by Graham Hutchings, Jens Rostrup-Nielsen and Yong-Wang Li. The book is based upon the courses developed for the SynCat Ac@demy over the period 2013-2017.**

# Publications and Conference Appearances 2017

## Core Publications of Syngaschem BV

[1] B. Caglar, M.O. Ozbek, J.W. Niemantsverdriet, C.J. Weststrate, Modeling the Surface Chemistry of Sugars: Glycolaldehyde on Rhodium (100) (vol 119, pg 22915, 2015), Journal of Physical Chemistry C, 121 (2017) 15489-15489.

[2] K. Holt, L. Jewell, H. Niemantsverdriet, L. Macheli, M. Shozi, G. Hutchings, T. Wezendonk, M. Bowker, R. Catlow, S. Adam, P.J. Kooyman, E. Hensen, J. Hayward, N. Coville, K.J. Weststrate, N. Fischer, A. Roldan, E. Redekop, E. van Steen, H. Friedrich, D.H. Kuo, H. Bandaru, L. Deeplal, A. Zivkovic, K. Naiker, C. Tucker, T.P.O. Mkhwanazi, D. Bahnemann, M. Neurock, A. Petersen, R.P. Forbes, T. Phaahlamohlaka, H. Schulz, D. Lennon, U. Olsbye, M. Wolf, S. Kondrat, P. Collier, X.H. Sun, Y. Zheng, A. Corma, E. Iglesia, T. Nyathi, D. Ma, M. Bremmer, M. Claeys, F. Kapteijn, Designing new catalysts for synthetic fuels: general discussion, Faraday Discussions, 197 (2017) 353-388.

[3] H. Niemantsverdriet, P. van Helden, E. Hensen, D. Lennon, K. Holt, G. Hutchings, M. Bowker, R. Catlow, M. Shozi, L. Jewell, M. Claeys, J. Hayward, N. Coville, N. Fischer, A. Roldan, E. Redekop, T. Gambu, L. Deeplal, T.P.O. Mkhwanazi, K.J. Weststrate, D. Bahnemann, M. Neurock, H. Schulz, D. Ma, S. Kondrat, P. Collier, A.K. Gupta, A. Corma, P. Akomeah, E. Iglesia, E. van Steen, N. de Leeuw, M. Wolf, T. van Heerden, Catalysis for Fuels: general discussion, Faraday Discussions, 197 (2017) 165-205.

[4] F.M. Sapountzi, J.M. Gracia, C.J. Weststrate, H.O.A. Fredriksson, J.W. Niemantsverdriet, Electrocatalysts for the generation of hydrogen, oxygen and synthesis gas, Progress in Energy and Combustion Science, 58 (2017) 1-35.

[5] C.J. Weststrate, J.W. Niemantsverdriet, Understanding FTS selectivity: the crucial role of surface hydrogen, Faraday Discussions, 197 (2017) 101-116.

[6] J. Gracia, Spin dependent interactions catalyse the oxygen electrochemistry, Physical Chemistry Chemical Physics, 19 (2017) 20451-20456.

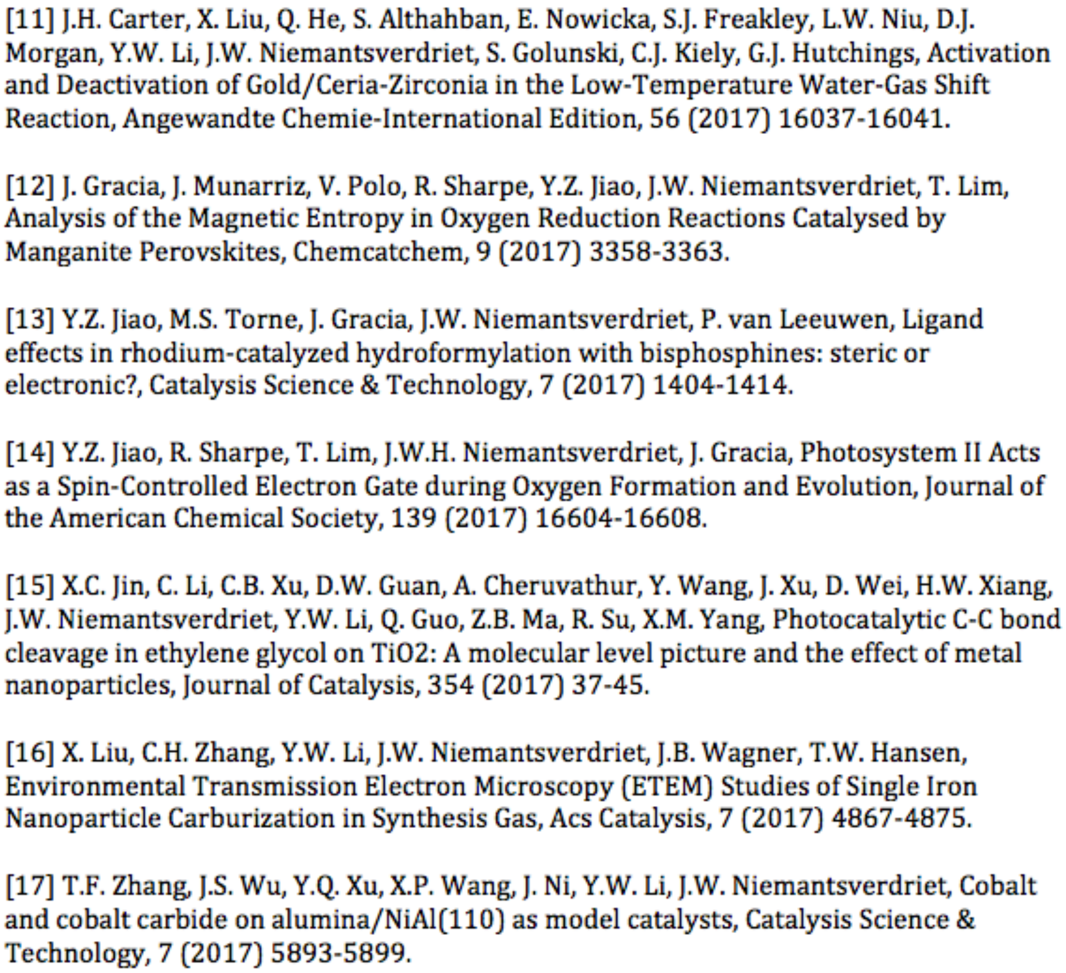
[7] M. Dad, R.J. Lancee, M.J. van Vuuren, J. van de Loosdrecht, J.W.H. Niemantsverdriet, H.O.A. Fredriksson, SiO2-supported Fe & FeMn colloids-Fischer-Tropsch synthesis on 3D model catalysts, Applied Catalysis a-General, 537 (2017) 83-92.

[8] F.M. Sapountzi, M.N. Tsampas, H.O.A. Fredriksson, J.M. Gracia, J.W. Niemantsverdriet, Hydrogen from electrochemical reforming of C1-C3 alcohols using proton conducting membranes, International Journal of Hydrogen Energy, 42 (2017) 10762-10774.

[9] C.J.M. van der Ham, F. Isik, T. Verhoeven, J.W. Niemantsverdriet, D.G.H. Hetterscheid, Activation pathways taking place at molecular copper precatalysts for the oxygen evolution reaction, Catalysis Today, 290 (2017) 33-38.

[10] B. Caglar, J.W. Niemantsverdriet, C.J. Weststrate, Modeling the surface chemistry of biomass model compounds on oxygen-covered Rh(100) (vol 18, pg 23888, 2016), Physical Chemistry Chemical Physics, 19 (2017) 893-893.

## Publications of SynCat@Beijing, with Syngaschem BV as co-affiliate



[11] J.H. Carter, X. Liu, Q. He, S. Althahban, E. Nowicka, S.J. Freakley, L.W. Niu, D.J. Morgan, Y.W. Li, J.W. Niemantsverdriet, S. Golunski, C.J. Kiely, G.J. Hutchings, Activation and Deactivation of Gold/Ceria-Zirconia in the Low-Temperature Water-Gas Shift Reaction, Angewandte Chemie-International Edition, 56 (2017) 16037-16041.

[12] J. Gracia, J. Munarriz, V. Polo, R. Sharpe, Y.Z. Jiao, J.W. Niemantsverdriet, T. Lim, Analysis of the Magnetic Entropy in Oxygen Reduction Reactions Catalysed by Manganite Perovskites, Chemcatchem, 9 (2017) 3358-3363.

[13] Y.Z. Jiao, M.S. Torne, J. Gracia, J.W. Niemantsverdriet, P. van Leeuwen, Ligand effects in rhodium-catalyzed hydroformylation with bisphosphines: steric or electronic?, Catalysis Science & Technology, 7 (2017) 1404-1414.

[14] Y.Z. Jiao, R. Sharpe, T. Lim, J.W.H. Niemantsverdriet, J. Gracia, Photosystem II Acts as a Spin-Controlled Electron Gate during Oxygen Formation and Evolution, Journal of the American Chemical Society, 139 (2017) 16604-16608.

[15] X.C. Jin, C. Li, C.B. Xu, D.W. Guan, A. Cheruvathur, Y. Wang, J. Xu, D. Wei, H.W. Xiang, J.W. Niemantsverdriet, Y.W. Li, Q. Guo, Z.B. Ma, R. Su, X.M. Yang, Photocatalytic C-C bond cleavage in ethylene glycol on TiO2: A molecular level picture and the effect of metal nanoparticles, Journal of Catalysis, 354 (2017) 37-45.

[16] X. Liu, C.H. Zhang, Y.W. Li, J.W. Niemantsverdriet, J.B. Wagner, T.W. Hansen, Environmental Transmission Electron Microscopy (ETEM) Studies of Single Iron Nanoparticle Carburization in Synthesis Gas, Acs Catalysis, 7 (2017) 4867-4875.

[17] T.F. Zhang, J.S. Wu, Y.Q. Xu, X.P. Wang, J. Ni, Y.W. Li, J.W. Niemantsverdriet, Cobalt and cobalt carbide on alumina/NiAl(110) as model catalysts, Catalysis Science & Technology, 7 (2017) 5893-5899.

## Books

1) **Concepts of Modern Catalysis and Kinetics (3rd Completely Revised and Enlarged Edition), Ib Chorkendorff and Hans Niemantsverdriet, Wiley-VCH (Weinheim), 2017**
2) **Scientific Leadership, Hans Niemantsverdriet and Jan-Karel Felderhof, DeGruyter (Berlin) 2017.**

## Contributions at Conferences

1) **"Understanding FTS selectivity, the crucial role of surface hydrogen", Kees-Jan Weststrate, Hans Niemantsverdriet, Catalysis for Fuels, Faraday discussion, Cape Town, January 24, 2017**
2) **"CO As an Active Spectator Species in Hydrocarbon Conversions Related to Fischer-Tropsch Synthesis", Kees-Jan Weststrate, Hans Niemantsverdriet, NAM 25, North American Catalysis Society Meeting , 6 june 2017**
3) **"Hydrogen production from short-chain alcohols using polymeric proton conductors", F.M. Sapountzi, M.N. Tsampas, H.O.A. Fredriksson, J.M. Gracia, J.W. Niemantsverdriet, 1st International Conference on Electrolysis (ICE 2017), Copenhagen, Dk, Jun 12-15, 2017**

## Summer Schools and Seminars at Institutes and Universities

4) **Scientific Leadership, general introduction (3 hours), Jan Karel Felderhof, Graham Hutchings, Hans Niemantsverdriet, c*change, University of Cape Town, January 26, 2017**

5) **Workshop Scientific Leadership (full day), Jan Karel Felderhof and Hans Niemantsverdriet, University of Cape Town, January 27, 2017**
6) **Workshop Scientific Leadership (half day), Hans Niemantsverdriet, University of the Free State, Bloemfontein, February 7, 2017.**
7) **"High vacuum techniques and model catalysts", Kees-Jan Weststrate, NIOK course "Characterization in catalysis research", University of Twente, 22 June 2017**
8) **Workshop Scientific Leadership (Full Day), Summer School Solids4Fun, Techical University of Vienna, July 5, 2017.**
9) **Catalysis and Future Electricity Technology – What is the Connection?, Hans Niemantsverdriet, Summer School Solids4Fun, Technical University of Vienna, July 6, 2017.**
10) **Catalysis and Future Electricity Technology – What is the Connection?, Hans Niemantsverdriet, Purdue University, West Lafayette, Indiana, USA, July 12, 2017.**
11) **"Surface Science investigations of the Fischer-Tropsch Reaction", Kees-Jan Weststrate, Hans Niemantsverdriet, Syngaschem – c*change workshop, 14 November 2017, Cape Town and 16 November, Bloemfontein**
12) **"XPS, High vacuum techniques and model catalysts", Kees-Jan Weststrate, 15 November, 2017, Cape Town**
13) **Kees-Jan acted as an opponent in PhD defense Marie Stromsheim, Norwegian University of Science and Technology, December 2017, Trondheim**
14) **"Model catalyst research at Syngaschem "Hans Fredriksson et al., Forschungszentrum Jülich, May 19, 2017**
15) **"Model catalyst preparation and testing", Hans Fredriksson et al., CritCat 12 month progress, Tampere, June 7, 2017**
16) **"WP5 - Catalyst development and optimization", Hans Fredriksson et al., CritCat 18 month progress, Brussels, December 6, 2017**

## Sponsoring

Syngaschem BV supports the Vincentre, a museum dedicated to the Dutch painter Vincent van Gogh in Nuenen, and the Classical Symphony Orchestra, The Philharmony Zuid-Nederland. On occasions, it sponsors local cultural events.

In 2017, it also supported the National Sports Contest of the Dutch Chemistry Students.

## Contact Information

syngaschem BV
synthesis gas chemistry
fundamental research projects

**Visiting address:** **De Zaale 20, 5612 AJ Eindhoven, The Netherlands**
**Postal address:** **PO Box 6336, 5600 HH Eindhoven, The Netherlands**
**Email addresses:** **info@syngaschem.com and office@syngaschem.com**
**Website:** **www.syngaschem.com**