syngaschem BV
synthesis gas chemistry
fundamental research projects

Syngaschem BV
Annual Report 2016

February 2017

Highlights

- Syngaschem moved from the Department of Chemical Engineering and Chemistry of the Eindhoven University of Technology TU/e to the Dutch Institute for Fundamental Energy Research (DIFFER), located at the TU/e campus. Here, Syngaschem occupies one laboratory and a large office, while it collaborates with the DIFFER Institute.
- Approval of a substantial research program together with DIFFER and TU/e – Physics funded jointly by the Netherlands Organisation for Scientific Research (NWO) and Syngaschem BV.
- Acquisition of EU-H2020 Funding in the CritCat Consortium.
- Publication of 21 papers together with SynCat@Beijing, and several international partners, such as Sasol Technology, the University of Capetown, the University of the Free State, TU/e, and Cardiff University.
- Syngaschem staff presented 5 invited lectures and 2 oral presentations at international conferences in the USA, China, Spain, Denmark and Germany.

SYNFUELS CHINA

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

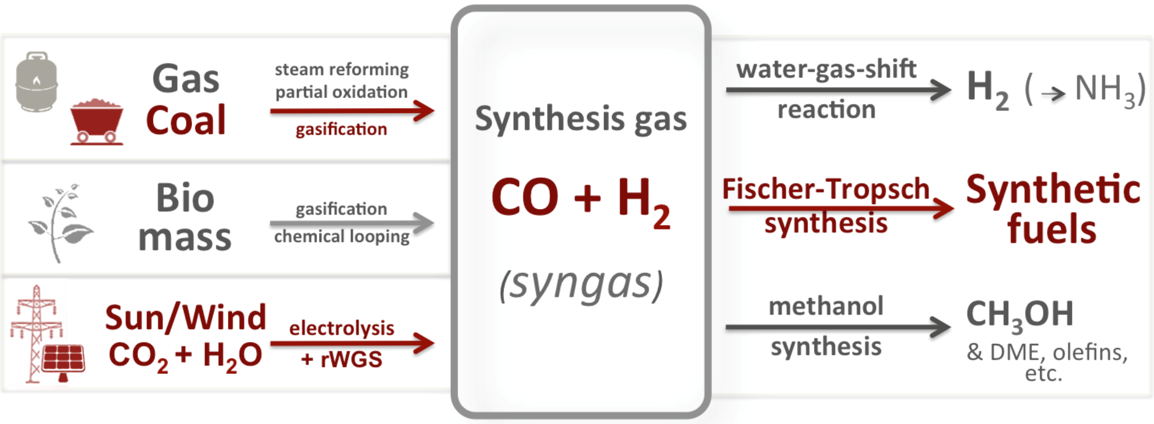
Syngaschem BV is Research Partner of Synfuels China Technologies Co., Ltd. and SynCat@Beijing

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 2016 at a glance

At the beginning of 2016, the preparations for SynCat@Beijing had largely been finished, with the laboratory in startup mode. The last big hurdle before research could be done at full scale was the ventilation, which was finished in February 2016. During the year, Prof Niemantsverdriet (11x) and Dr Weststrate (2x) visited Beijing regularly, while also Ir Felderhof visited two times for coaching and scientific leadership development courses.

At its home base in Eindhoven, Syngaschem BV had moved out of the old TU/e laboratory in the Departmentment of Chemical Engineering and Chemistry to the new DIFFER building in December 2015, and 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. Fortunately, some of the microreactor equipment at TU/e could still be used during parts of 2016, for which we gratefully acknowledge the research group of Prof Emiel Hensen.

The somewhat limited availability of instrumentation enabled the staff to publish much of the previous research, with the result that Syngaschem staff published or coauthored a record number of 21 papers in 2016. A remarkable highlight was the publication of a lengthy review on electrocatalysts for the generation of H_2 and O_2 from water, which appeared as open access paper in Progress in Energy and Combustion Science, a journal with an impact factor of 16.784! We refer to the publication list at the end of this report.

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 11 visits to SynCat@Beijing in 2016, and spent almost 30% of his time in Beijing. 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.
- In February, Kees-Jan Weststrate, Hans Fredriksson and Gilbère Mannie from SynCat@Beijing had a joint synchrotron session in Aarhus of almost two weeks.

- In August, Dr Jose Gracia visited Syngaschem BV to discuss the future strategy of the electrolysis research on both sides, as well as some practical issues on electrolytic testing.
- Syngaschem Advisor, Prof Mike Bowker, visited SynCat@Beijing twice in July and in November 2016, to discuss progress with the SynCat staff, and to help review the research program at SynCat@Beijing.
- Ir Jan Karel Felderhof visited SynCat@Beijing twice for a week, to coach the staff members, and guide them in developing their career plans.
- Six publications appeared in 2016 with joint affiliations of SynCat@Beijing and SynCat@DIFFER, with Jose Gracia, Tingbin Lim, Ryan Sharpe, Yunzhe Jiao, Ren Su and being the authors from the SynCat@Beijing side, and all Syngaschem staff on the Dutch side.

Syngaschem Advisors

In 2016, Syngaschem staff benefitted from several meetings with Prof Mike Bowker of the Cardiff Catalysis Institute, held in Eindhoven in June, in Beijing in July, and in Cardiff in March and November. In August, Hans Niemantsverdriet had a meeting with Dr Jens Rostrup Nielsen on strategic developments, in Virum, Denmark. We are grateful to the many valuable contributions that our scientific advisors have made over the years.

Syngaschem Staff in 2016

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 (0.8 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		
Ms Yibin Bu	PhD Student China Scholarship Council	
Mr Emad Dad	PhD Student; completed PhD in June 2016	
Mr Marc Bonte	Student Fontys University of Applied Sciences	

Successful Grant Applications

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 will remain as our first and foremost 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. The following successes have been booked:

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, and 75.000 Euro in 2016. Though modest, it enables 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.

EU H2020 Grant: CritCat

In 2015, Syngaschem BV was invited to join a European Consortium named CritCat, to qualify for a grant from the European Union under the roof of the Horizon 2020 program. CritCat intends to use its capabilities to control cluster sizes of nanoparticles and validate theoretically predicted performance in catalysis. DFT modelling and prediction together with the concept of machine learning should lead to noble-metal free catalysts.

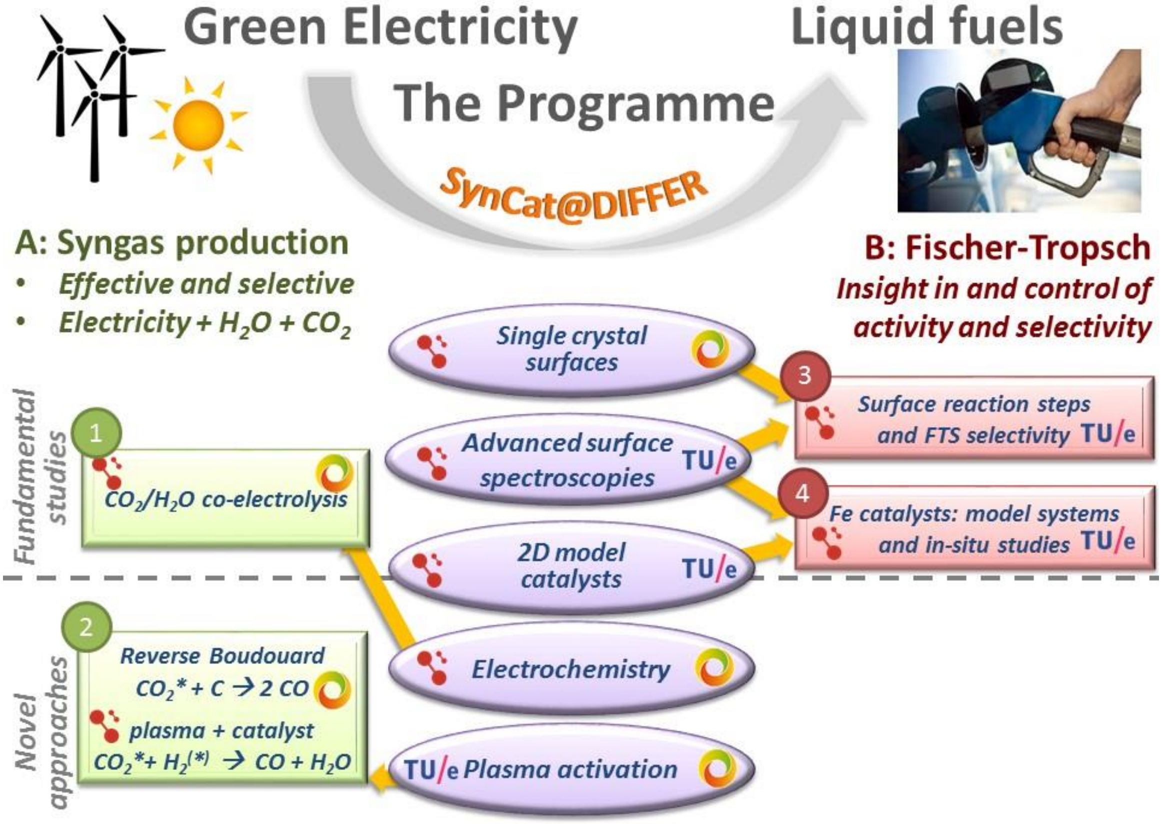
CritCat Consortium	Key expertise
Dr J Akola, TU Tampere, Finland (Consortium leader)	DFT-modeling of metal nanoparticles
Prof K Laasonen, Aalto University, Finland	DFT modeling, including electrocatalysis
Dr D Gao, Nanolayers Ltd., UK	Machine learning algorithms
Prof R Palmer, University of Birmingham, UK	Mass-selective synthesis of nanoparticles
Dr S Vinati, Tethis S.p.a., Italy	Size controlled nanoparticles
Prof R Dunin-Borkowski, FZ Jülich, Germany	Transmission Electron Microscopy
Dr A Wain, National Physical Laboratory, UK	Electrochemical Characterization
Dr Y Kolenko, Iberian Nanotech Laboratory, Portugal	Material synthesis and Applied Electrochemistry
Syngaschem BV, Netherlands	Electro and model catalysis

The Critcat consortium went successfully through a two-stage evaluation and was selected for funding, in spite of typical success rates being 10% only. According to the EC grant agreement No. 686053, titled "Towards Replacement of Critical Catalyst Materials by Improved Nanoparticle Control and Rational Design", Syngaschem shares 500.000 Euro of the total budget of 4.3 million Euro over three years. These resources are dedicated to research on electrocatalytic reactions and nanoparticle synthesis and testing. Dr Sapountzi will lead Syngaschem's activities in electrochemistry, Dr Fredriksson takes care of catalyst testing, and Mr. Vaccaro contributes to the exploitation management of the CritCat consortium. The official start date was June 1, 2016, but Syngaschem's major activities for the program start mainly in 2017.

NWO-CHIPP Program SynCat@DIFFER

Syngaschem, DIFFER and a spectroscopy group at the Department of Applied Physics at TU/e obtained a significant subsidy from the Netherlands Organisation of Scientific Research (NWO). The initiative formed the basis for collaboration with DIFFER, on which Syngaschem BV could establish itself at the DIFFER premises. This “Chemical Industrial Private Partnership” or ChIPP project is intended for public-private co-operation of at least one company with at least two knowledge institutes. Projects are funded for 50% by the industry and for 50% by the Netherlands Organization for Research NWO, and receive about 10% extra subsidy from governmental funds. The total budget is 1.65 Million Euro.

The program is summarized in the scheme below. It enables in total five postdoc and PhD positions as well as substantial investment in electrochemistry and surface science equipment, while projects 1, 3, and 4 come directly out of Syngaschem’s research plans. Although the director of DIFFER, Prof dr R. van de Sanden is formally principal investigator, Dr Kees-Jan Weststrate serves as the program coordinator.

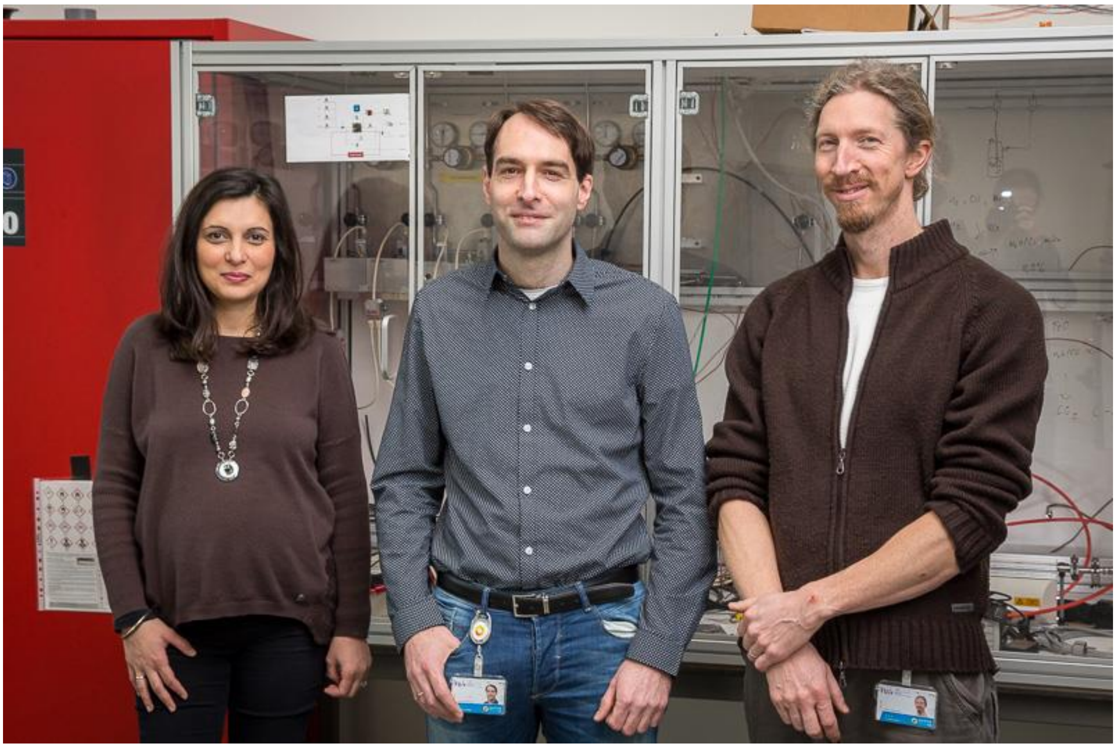


Research Plan of the CHIPP Proposal SynCat@DIFFER which has been granted by the Netherlands Organisation for Scientific Research NWO; this program forms the cornerstone of the Syngaschem – DIFFER – TU/e collaboration from 2016 onwards and enable us to employ several PhD students in the research.

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 will come on stream in 2017.
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. During 2017, a collaboration with Dr Peter Thüne at Fontys University of Applied Sciences will start, where students will be involved in the synthesis and testing of catalysts.



From left to right: Dr Foteini Sapountzi, Dr Kees-Jan Weststrate, Dr Hans Fredriksson

Research Highlights 2016

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

We explored the surface chemistry of 1-olefins up to 1-heptene, and the influence of CO on the stability of various intermediates to get a more general view on how CO affects chain growth intermediates longer than C3. Figure 1 shows the experimental results for 1-butene, studied using temperature programmed desorption (a), and infrared absorption spectroscopy (b). In analogy to propene, a saturated layer of chemisorbed 1-butene decomposes into a mixture of 1-butyne (C_2H_5-C-CH, major) and butylidyne (C_3H_7-C, minor) when heated to 200 K. Further heating in vacuum leads to decomposition of minority butylidyne to a pure butyne layer at 300 K. Surface hydrogens produced in the butene → butyne reaction desorb below 320 K, as shown in (a).

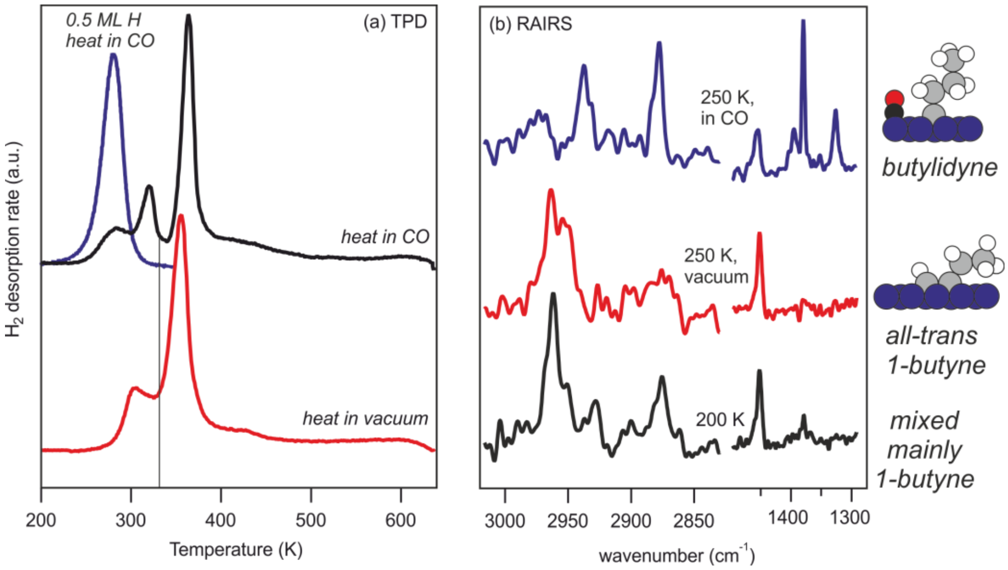


Figure 1: (a) Comparing H_2 desorption of 1-butene adsorbed on Co(0001) during heating in vacuum (red) and in the presence of CO (black). (b) IR absorption spectra at 200 K, and at 250 K after heating in vacuum (red) and in CO (blue).

When the mixed layer formed at 200 K is heated in the presence of CO the low temperature H_2 peak splits into two components, where the low temperature peak corresponds to only one out of the 8 hydrogen present in the 1-butene precursor. The peak temperature coincides with that of desorption of surface-bound hydrogen under the influence of CO [shown as ref. in (a)]. This indicates rehydrogenation of butyne to butylidyne under the influence of the CO co-adsorbate. Infrared absorption studies, shown in (b), confirm this view. The spectrum after heating of the mixed butyne-butylidyne layer (formed at 200 K) to 250 K in vacuum shows the asymmetric CH_3 bending and stretching modes (1460 cm^{-1}, 2960 cm^{-1}), attributed to a butyne in an all-trans configuration. Instead, heating to 250 K in the presence of CO shows a very different spectrum, with characteristic bands attributed to butylidyne, with CH_2 stretching modes at 2930 cm^{-1} and the symmetric CH_3 modes at 2870 cm^{-1} and 1370 cm^{-1}. Similar results were obtained for longer 1-alkenes.

The present study shows that the surface chemistry of hydrocarbonaceous adsorbates is strongly affected by the presence of CO adsorbates. Co-adsorbed CO stabilizes in particular the alkylidyne adsorbate over the alkyne adsorbate, the most stable C_xH_y adsorbate on Co(0001) in the absence of CO. This experimental finding emphasizes that studies of hydrocarbon chemistry in the context of Fischer-Tropsch synthesis should explicitly consider influence of CO, expected to be present in abundance under reaction conditions.

Electrocatalytic processes for storing renewable energy in chemical bonds
(Dr Foteini Sapountzi)

Our extensive literature review “Electrocatalysts for the generation of hydrogen, oxygen and synthesis gas” recently published in “Progress in Energy and Combustion” has served to guide Syngaschem’s research agenda in the field of Syngas-production by water electrolysis and will continue to do so in 2017.

Hydrogen from electrochemical reforming of C1-C3 alcohols using H^+ conducting membranes

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. In collaboration with DIFFER and Synfuels China we studied the production of hydrogen through the electro-reforming of short-chain alcohols (methanol, ethanol, iso-propanol) and their mixtures.

Gas diffusion electrodes with high surface area were interfaced to a polymeric H^+ conductor and the assembly was introduced in an aqueous dual chamber electrochemical reactor. This reactor offers a simpler design and lower cost compared to the typical PEM electrolyzers, thus this system is more appropriate for fundamental investigations. Moreover, it allows the utilization of a standard Ag/AgCl reference electrode, which enables us to monitor the individual anodic and cathodic overpotentials.

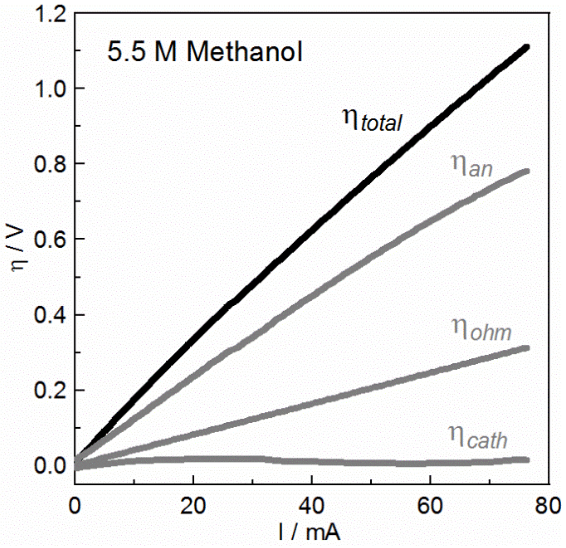


Figure 2: Effect of the cell current on the total cell overpotential and on the individual anodic, cathodic and ohmic overpotentials. Analyte: 5.5M CH_3OH+0.2M H_2SO_4.

Figure 2 depicts the deconvolution of the potential losses during the electrochemical reforming of methanol. The performance of the cell is mainly limited by the sluggish kinetics of the alcohol electrooxidation reaction which takes place at the anode. It was found that the anodic overpotential becomes larger as the number of C-atoms in the alcohol increases, while when using alcohol mixtures, the cell performance is dictated by the largest alcohol.

An article manuscript has been already drafted and is planned to be submitted for publication. Future plans for the continuation of this project are (i) the use of n-propanol for investigating mechanistic details, (ii) the use of alternative catalysts (in the frame of Critcat project) and of high surface area Ti-based supports (collaboration with DIFFER), (iii) the use of OH^- conducting polymeric electrolytes (supplied by Tokuyama).

Evaluation of electrocatalysts for PEM water electrolysis

In the framework of Critcat, rationally designed noble metal-free electrode material will be tested under industrially relevant conditions. A set-up has been designed which consists of four main parts; (i) the gas supply unit comprised of the gas cylinders, thermostated gas saturators, mass-flow controllers, valves and heated tubes, (ii) the reactor unit which consists of a state-of-the-art PEM electrochemical cell (Dupont) together with its heating elements, (iii) the characterization unit which includes the electrochemical characterization tools and accessories and the instrumentation for the gas analysis of the reaction products, (iv) the control unit for regulating the operational parameters.

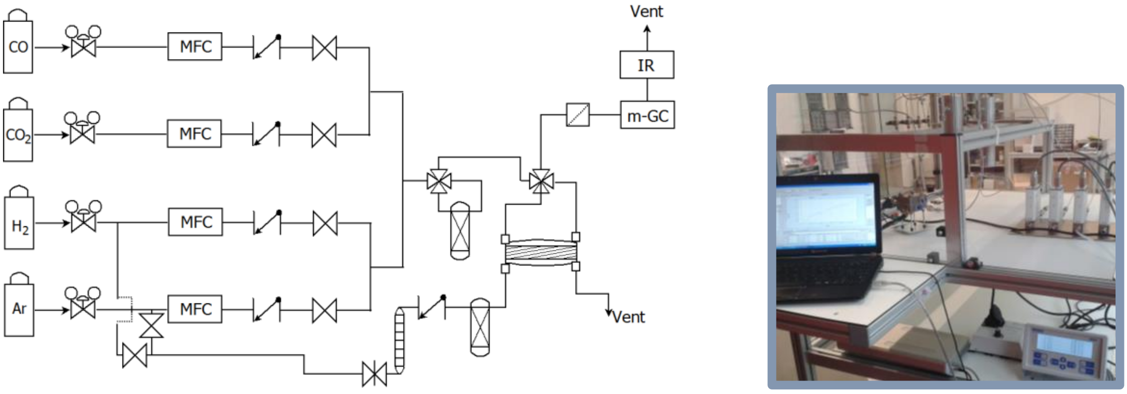


Figure 3: Left: Process flow diagram of the testing unit. Right: Photograph of the experimental setup.

Electrocatalysis – Oxygen Evolution over $LaCoO_3$

(Dr Hans Fredriksson and Dr Foteini Sapountzi)

In the framework of a collaboration with Synfuels China, efforts to increase the precision and reliability of electro-catalytic activity data have been made. To avoid electrode preparation steps such as drop casting a C-support with an ink based on perovskite powder, pulsed laser deposition (PLD) was used in a collaboration with the technical university in Twente (UT) to deposit thin homogeneous perovskite films as the working electrodes. Although the reproducibility was only slightly improved, the activity of the PLD deposited electrodes showed an activity roughly one order of magnitude larger than the perovskite powder electrodes, when normalized on catalyst mass. As shown in Figure 4, thin film electrodes perform better at high current densities while the powder electrodes require a lower voltage for the reaction to start. This observation suggests that the contact between the catalyst and the support plays a significant role for the oxygen evolution performance under our experimental conditions.

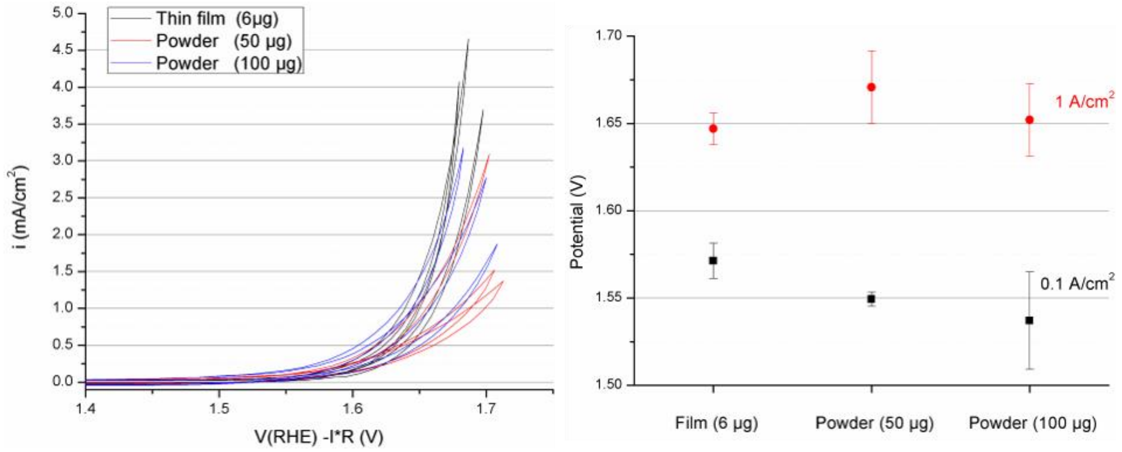


Figure 4: $LaCoO_3$ catalysts tested for OER. Left: CV scans for the three tested catalysts (black) PLD deposited film and (red, blue) powder catalysts with two different loadings. Right: the potentials required for reaching 0.1 and 1 A/cm^2 during the forward scan for the same three catalysts.

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). An in-house developed micro reactor with in-situ UV-vis spectroscopy was 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.

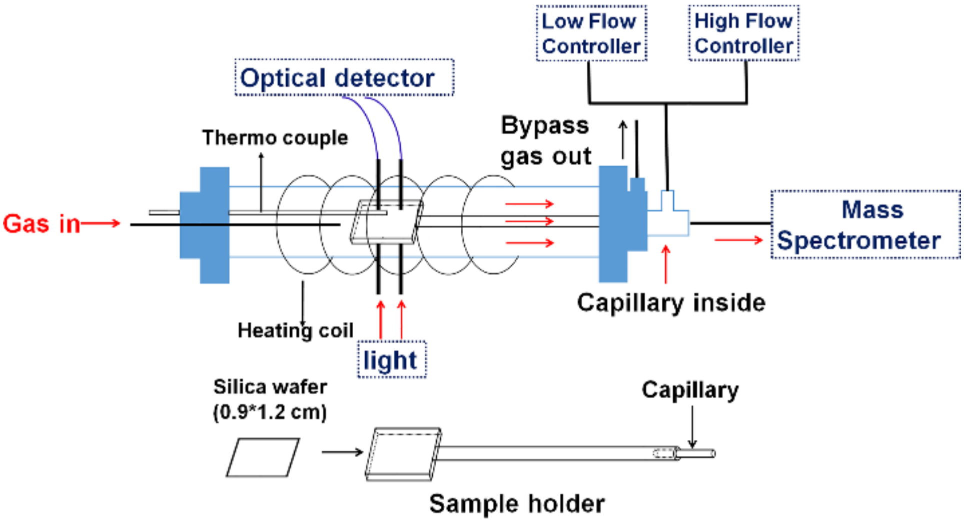


Figure 5: Micro reactor with in-situ UV-vis and mass spectroscopy for testing of model catalysts

Testing flat model catalysts of Cu and Cu/CeO_x under conditions relevant for methanol synthesis and WGS in combination with XPS revealed that Cu promotes the reduction of Ce^{4+} to Ce^{3+} (see Figure 6). At the same time, Ce^{3+} promotes the dissociation of CO_2 and H_2O, which in turn leads to oxidation of metallic Cu to Cu^{1+}. This work, a collaboration between TU/e and Syngaschem BV, has been published in ACS catalysis.

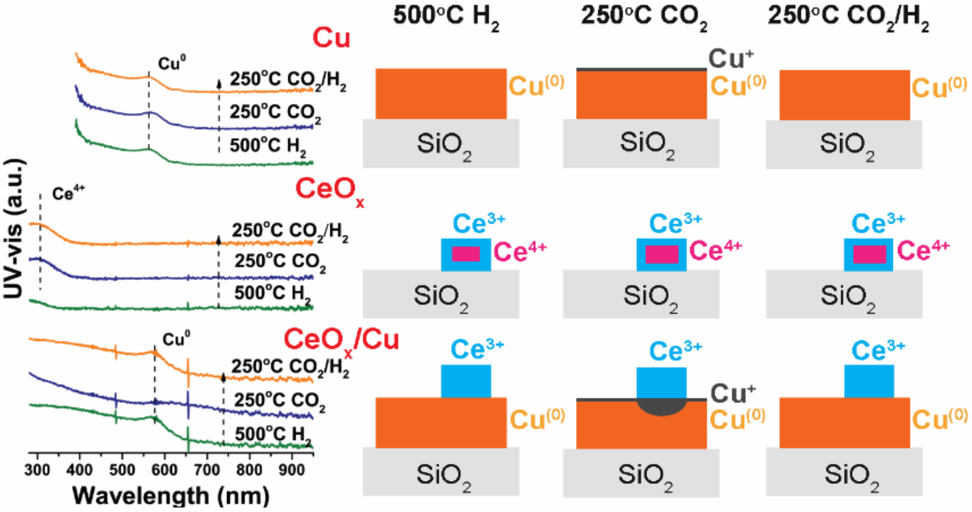


Figure 6: UV-vis spectra of Cu, CeO_x and Cu/CeO_x catalysts after reduction in H_2 and subsequent exposure to CO_2 and CO_2/H_2. The schematic figure shows the phase changes in the catalysts upon the changes in gas composition

Model catalysts for FTS

A three dimensional Mn promoted Fe catalyst consisting of pre-formed monodisperse nanocolloids, supported on non-porous SiO_2 microspheres was developed. With this model catalyst Fischer-Tropsch synthesis experiments under industrially relevant conditions became possible through increased surface areas, while the original advantages of low-surface area two dimensional systems (access to careful characterization by TEM, SEM, XPS, XRD, ATR-IR and ICP) were kept. We found that Mn alters the catalyst's selectivity and improves its stability. The characterization shows encapsulation of the active material in carbon layers, some sintering and catalyst reduction/FeC_x formation during use. This work, a collaboration between TU/e, Sasol and Syngaschem, has been submitted for publication in Applied Catalysis A.

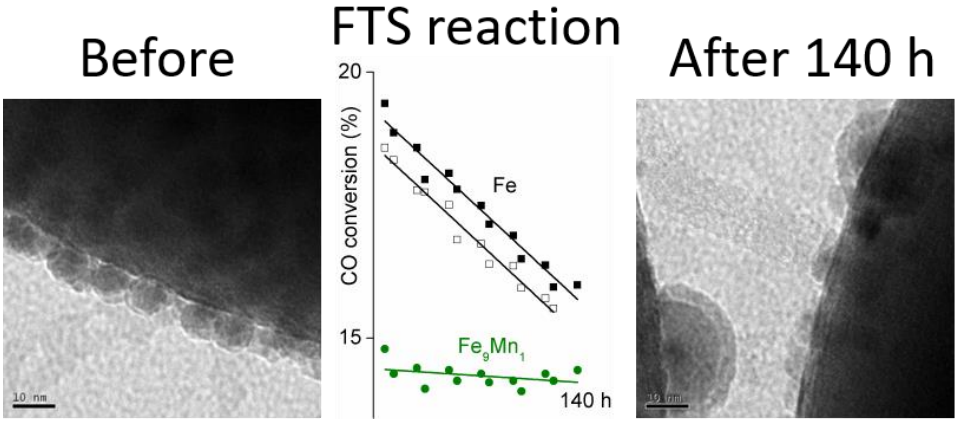
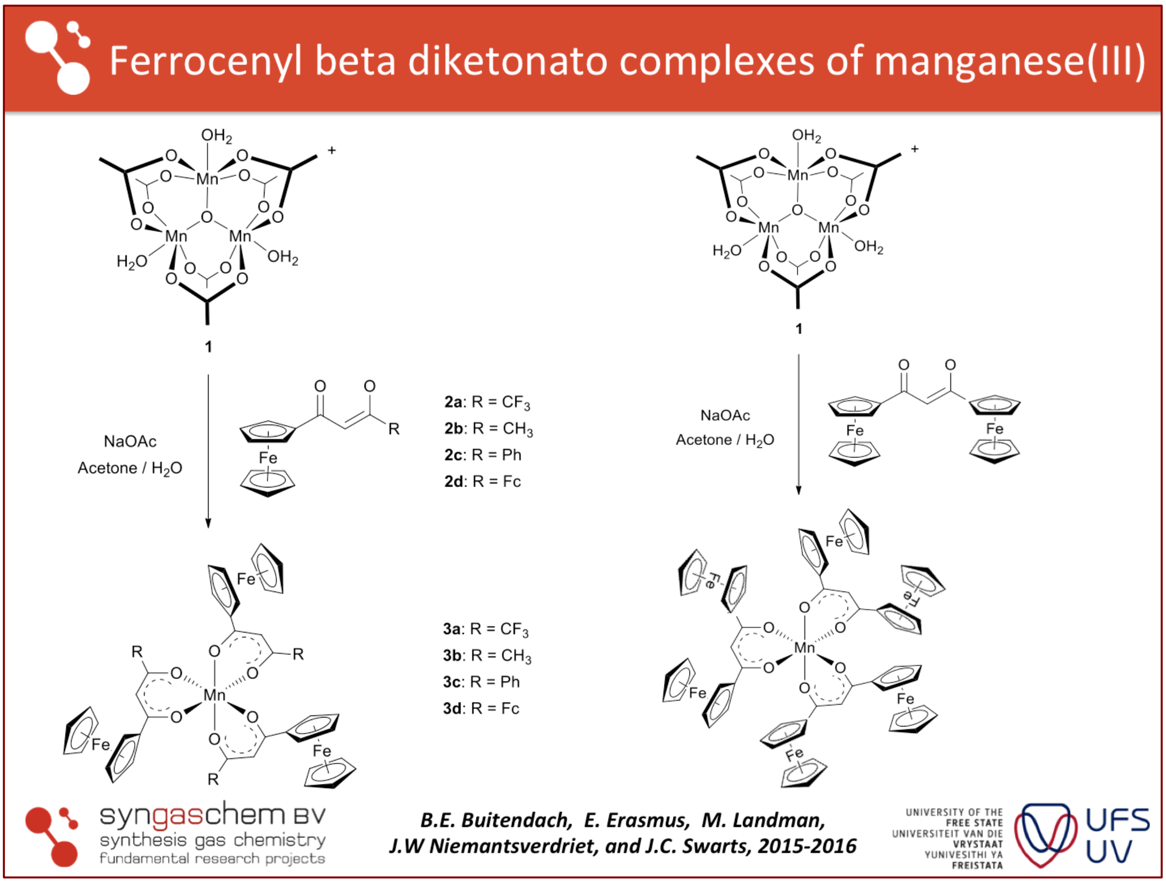
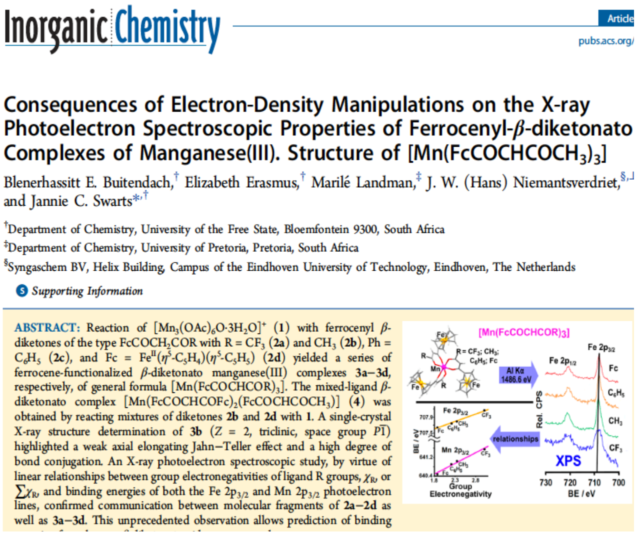


Figure 7: Three-dimensional model catalyst consisting of monodisperse Fe nano colloids on SiO_2 before and after 140 h of testing under industrial FTS conditions. The graph shows the change in CO conversion during for two identical unpromoted Fe catalysts and a more stable Mn-promoted catalyst.

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.


Inorganic Chemistry

Article

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Consequences of Electron-Density Manipulations on the X-ray Photoelectron Spectroscopic Properties of Ferrocenyl-β-diketonato Complexes of Manganese(III). Structure of [Mn(FcCOCHCOCH$_3$)$_3$]

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Supporting Information

ABSTRACT: Reaction of $[Mn_3(OAc)_6O\cdot 3H_2O]^+$ (1) with ferrocenyl β-diketones of the type FcCOCH$_2$COR with R = CF$_3$ (2a) and CH$_3$ (2b), Ph = C$_6$H$_5$ (2c), and Fc = $Fe^{II}(\eta^5\text{-}C_5H_4)(\eta^5\text{-}C_5H_5)$ (2d) yielded a series of ferrocene-functionalized β-diketonato manganese(III) complexes 3a–3d, respectively, of general formula [Mn(FcCOCHCOR)$_3$]. The mixed-ligand β-diketonato complex [Mn(FcCOCHCOFc)$_2$(FcCOCHCOCH$_3$)] (4) was obtained by reacting mixtures of diketones 2b and 2d with 1. A single-crystal X-ray structure determination of 3b (Z = 2, triclinic, space group $P\overline{1}$) highlighted a weak axial elongating Jahn–Teller effect and a high degree of bond conjugation. An X-ray photoelectron spectroscopic study, by virtue of linear relationships between group electronegativities of ligand R groups, χ_R, or $\sum\chi_R$, and binding energies of both the Fe 2p$_{3/2}$ and Mn 2p$_{3/2}$ photoelectron lines, confirmed communication between molecular fragments of 2a–2d as well as 3a–3d. This unprecedented observation allows prediction of binding

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. Two joint publications appeared on the reduction promotion of cobalt by noble metals.

Publications and Conference Appearances 2016

Core Publications of SynCat@DIFFER and SynCat@Beijing

1) “Electrocatalysts for the generation of hydrogen, oxygen and synthesis gas”
   Foteini M. Sapountzi, Jose M. Gracia, C.J. (Kees-Jan) Weststrate, Hans O.A. Fredriksson, J.W. (Hans) Niemantsverdriet, *Progress in Energy and Combustion Science* **58** (2017) 1
2) “Reflections on the Fischer-Tropsch synthesis: Mechanistic issues from a surface science perspective”
   C.J. Weststrate, P. van Helden, J.W. (Hans) Niemantsverdriet, *Catalysis Today* **275** (2016) 100
3) “Spectroscopic insights into cobalt-catalyzed Fischer-Tropsch synthesis: A review of the carbon monoxide interaction with single crystalline surfaces of cobalt"
   C.J. Weststrate, J. van de Loosdrecht, J.W. Niemantsverdriet, *J. Catal.* **342** (2016) 1
4) “Role of ZnO and CeO_x in Cu-Based Model Catalysts in Activation of H_2O and CO_2 Dynamics Studied by in Situ Ultraviolet–Visible and X-ray Photoelectron Spectroscopy”
   Yibin Bu, C. J. Weststrate, J. W. Niemantsverdriet, and Hans O. A. Fredriksson, *ACS Catal.* **6** (2016) 7994
5) “Cu Model Catalyst Dynamics and CO Oxidation Kinetics Studied by Simultaneous in Situ UV–Vis and Mass Spectroscopy"
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Co-authored Publications of Syngaschem staff related to earlier work and collaborations

11) "Detangling Catalyst Modification Reactions from the Oxygen Evolution Reaction by Online Mass Spectrometry",
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12) "The effect of C–OH functionality on the surface chemistry of biomass-derived molecules: ethanol chemistry on Rh(100)"
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    B. Caglar, J.W. Niemantsverdriet, and C.J. Weststrate, *Phys. Chem. Chem. Phys.* **18** (2016) 23888
14) "Hydrogen spillover in the Fischer–Tropsch synthesis: An analysis of gold as a promoter for cobalt–alumina catalysts",
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16) "Hydrophilic Interaction Between Low-Coordinated Au and Water: H_2O/Au(310) Studied with TPD and XPS"
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    C.J. Weststrate, P. van Helden, J. van de Loosdrecht, J.W. Niemantsverdriet, *Surf. Sci.* **648** (2016) 60
18) "Oxygen Adsorption and Water Formation on Co(0001)"
    A.C. Kizilkaya, J.W. Niemantsverdriet, and C.J. Weststrate, *J. Phys. Chem. C* **120** (2016) 4833
19) "Ammonia Adsorption and Decomposition on Co(0001) in Relation to Fischer–Tropsch Synthesis"
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20) "Nano-heaters: New insights on the outstanding deposition of dielectric energy on perovskite nanoparticles"
    J. Gracia, M. Escuin, R. Mallada, N. Navascues, J. Santamaria, *Nano Energy* **20** (2016) 20
21) “Early stages of catalyst aging in the iridium mediated water oxidation reaction”
    D.G.H. Hetterscheid, C.J.M van der Ham, O. Diaz-Morales, M.W.G.M. Verhoeven, A. Longo, D. Banerjee, J.W. Niemantsverdriet, J.N.H. Reek, and M.C. Feiters, Phys. Chem. Chem. Phys. 18 (2016) 10931.

Contributions at Conferences

1) "Surface science investigations of the Fischer-Tropsch reaction on cobalt" (invited lecture), Kees-Jan Weststrate, Hans Niemantsverdriet, 251st ACS National Meeting, San Diego, California, Mar 13-17, 2016
2) "Presenting Science"
Hans Niemantsverdriet, TU Munich Graduate Academy, Burghausen, Germany, Jun 5-8, 2016
3) "Hydrocarbon chemistry on cobalt: surface science investigations of the FT chain growth mechanism"
Kees-Jan Weststrate, NGSC 11, Tromsø, Norway, Jun 5-9, 2016
4) "Why Fischer-Tropsch synthesis needs carbon monoxide: the role of CO in the FTS chain growth mechanism"
Kees-Jan Weststrate, Hans Niemantsverdriet, ICC-2016, Beijing, China, Jul 3-8, 2016
5) "Syngas as Essential Ingredient of Electricity Storage Technology: Electrolysis and Fischer-Tropsch Synthesis" (plenary lecture)
Hans Niemantsverdriet, Jose Gracia and Kees-Jan Weststrate, Post-symposium on Catalysis for Syngas and Methanol Conversion of ICC-2016, Huairou/ Beijing, China, Jul 10-11, 2016
6) "Model Systems for addressing Fundamental and Practical Questions in Heterogeneous Catalysis" (invited lecture)
Hans Niemantsverdriet, CINF Summer School 2016 – Reactivity of nanoparticles for more efficient and sustainable energy conversion – IV, Gilleleje, Denmark, Aug 8-13, 2016
7) "Syngas and Fischer-Tropsch Synthesis for Energy-Dense Liquid-Fuel Production in Energy Technology" (plenary lecture)
Hans Niemantsverdriet, Jose Gracia and Kees-Jan Weststrate, CCESC 2016 Conference, Madrid, Spain, Sep 7-9 2016

Seminars at Institutes and Universities

Hans Niemantsverdriet gave several seminars at universities:

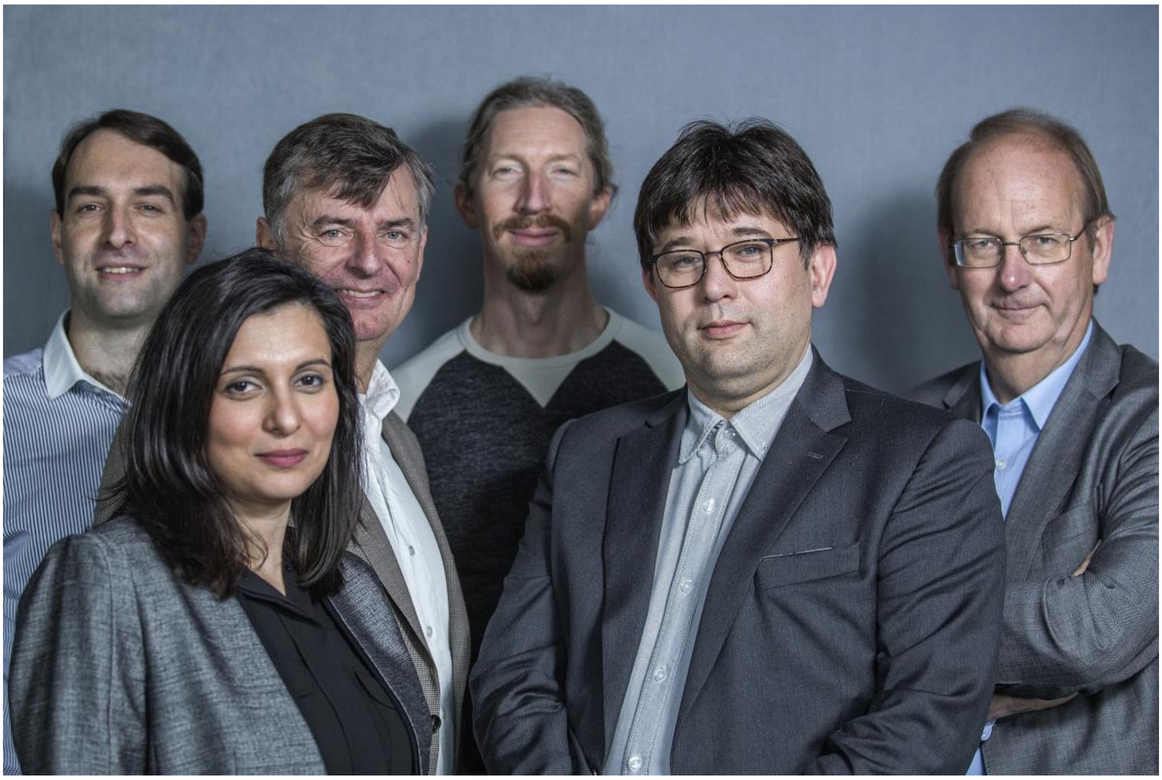
- Peking University, Jan 14, 2016 - Fischer-Tropsch Chemistry
- SynCat@Beijing, Feb 22, 2016 – Reaction Rate Theory
- ETH Zurich, Feb 30, 2016 – Fischer-Tropsch Chemistry
- Jiangsu University, Oct 21, 2016 – Oxygen Evolution and Fischer-Tropsch Chemistry
- Cardiff University, Nov 29+30, 2016 – Scientific leadership; presenting science

Sponsoring

Syngaschem BV sponsored the Fischer-Tropsch symposium at the 251st ACS National Meeting, San Diego, California, Mar 13-17, 2016.

Syngaschem commits to regular support of 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 2016, Syngaschem BV supported the impressive action of Dutchman Mark Koelen from Eindhoven: Mr. Koelen cycled more than 20.000 km through the Americas to reach Olympic City Rio de Janeiro in order to generate public attention to his charitable project benefitting impoverished children living in the favelas.



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