

# Syngaschem BV Annual Report 2018

March 2019



Syngaschem BV is Research Partner of SynCat@Beijing; it receives base funding from Synfuels China Technology Co., Ltd, Beijing-Huairou.



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## Highlights

- 2 Major Research Programs: namely the NWO-sponsored CHIPP project together with the DIFFER Institute and the TU/e, with 50/50% co-funding by NWO and Syngaschem BV, enabled by base funding from Synfuels China, and the Horizon 2020 CritCat Consortium with 9 European partners, funded by the EU-H2020 program.
- **17** Publications: 5 papers on Syngaschem-based or initiated research, 7 in collaboration with SynCat@Beijing, and 5 more in the pipeline.
- 34 Scientific Presentations: Syngaschem staff gave 14 oral presentations at international conferences and universities in the USA, South Africa, China, Denmark, Poland and Italy and another 11 at workshops and university visits. In addition they presented 9 posters at conferences.
- Exchange Visit to Beijing: all SynCat@DIFFER staff visited SynCat@Beijing in April, and participated in a symposium, laboratory tour and individual discussion meetings.
- Syngaschem BV 5 years: to celebrate, Syngaschem BV sponsored several scientific meetings and placed a special advertisement in the program books.

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### 1. Introduction: What is Syngaschem BV?

Syngaschem BV is a Dutch private research enterprise founded in collaboration with Synfuels China Technology in China. Together they established a laboratory for fundamental research, entitled SynCat@Beijing, which took off in 2015. Syngaschem was founded in 2013 to take care of recruitment of staff and planning of research programs 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. Syngaschem employs three research scientists and accommodates several students, while it is also active in providing scientific leadership training.

## 2. Vision and Mission: Energy Storage and CO<sub>2</sub> Avoidance

The SynCat laboratories operate on the vision that hydrogen and synthesis gas  $(CO + xH_2)$  are crucial intermediates in clean energy technologies for the future, in many parts of the world. Synthesis gas – or in short 'syngas' – can be obtained from traditional fossil sources, as well as from biomass and from electricity in combination with water and sources of carbon, see the scheme below. With the advent of renewable electricity from wind and solar energy, which is inherently intermittent, syngas 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, even more so if all electric power used in the process itself would come from renewable sources as well.



The mission of Syngaschem BV is to obtain fundamental understanding behind the production of syngas 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, and on surface science and spectroscopy for understanding of CO hydrogenation reactions, often in combination with molecular modeling.

## 3. Research Program in 2018

As a result of the generous base funding by Synfuels China and the additional subsidies (see Text Box), the research program continued to consist of three major subjects in 2018:

 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 Cape Town (Prof Michael Claeys and Dr Nico Fischer) focuses on the selectivity of FTS Catalysts for special products, and the stability of catalysts over time, and it has been running successfully in 2018. We will continue to fund these projects in 2019 as well.

#### **Overview Funding Sources**

- Base funding from Synfuels China Technology Co. Ltd.
- NWO CHIPP Subsidy for a 4-years research program together with the DIFFER Institute and TU/e (total budget approximately 1.6 M€)
- European Union Horizon 2020 funding for the CritCat program (total amount 500 k€)
- Annual subsidy on labour cost in tax deductions from the Ministry of Economic Affairs (WBSO)
- 2) Electrolysis of Water and CO<sub>2</sub> 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 under acid and alkaline conditions. We are gradually shifting attention towards zero-gap configuration electrolysis, using anion exchange membranes (collaboration with Prof Hristo Penchev, Bulgarian Academy of Sciences). Within the CritCat consortium the emphasis is on testing novel formulations based on computational predictions for H<sub>2</sub> evolution. In a collaboration with the University of the Free State in South Africa (Dr Blener Buitendach and Prof Jannie Swarts), we study cluster derived iridiumruthenium systems for oxygen evolution reactions. This successful project will continue in 2019 as well.
- 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<sub>2</sub> activation with optical plasmon resonance techniques inside microreactors. In the framework of the CritCat Project, catalysts are tested for H<sub>2</sub> formation by ammonia decomposition and for decomposition of volatile organic compounds. Within this project, a PhD thesis on pulsed operation in microreactors (collaboration with Prof.Dr. Ton Backx, TU/e) was completed in 2018 by Mr Zhenghang Zhu, and will be defended in 2019.

Name	Major Activities	Project Funding
Dr Hans Fredriksson (0.9 fte)	In situ spectroscopy, micro reactors, CO <sub>2</sub>	EU - CritCat project
Dr Foteini Sapountzi (0.8 fte)	Electrochemistry; electrolysis	EU - CritCat project
Dr Kees-Jan Weststrate (0.9 fte)	Surface Science; Fischer-Tropsch Chemistry	SynCat@DIFFER
Mr Antonio Vaccaro (0.1 fte)	Administration	
Ir Jan Karel Felderhof (0.1 fte)	Director Strategy, Organisation, HR Development; SynCat Ac@demy	
Prof dr Hans Niemantsverdriet (0.6 fte)*	Director Syngaschem BV (* in 2018: 0.3 fte due to illness)	
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	
Ms Sharleen Babouram)	MSc student (Fontys Univ of Applied Sciences); EU-CritCat project	
Mr Yun Ku (Michael) Hu	MSc student (Fontys Univ of Applied Sciences); EU-CritCat project	
Ms Jacky Olinga	MSc student (Fontys Univ of Applied Sciences); EU-CritCat project	

## 4. Syngaschem Staff and Students in 2018

## 5. Research 2018

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

Two projects feature in the Syngaschem Laboratories in the context of the SynCat@DIFFER programme. In the first we use single crystal surfaces of cobalt to study elementary steps of FTS chain growth. During 2018 we visited the synchrotron in Trieste, Italy, for high resolution fast XPS measurements. The high signal intensity and high resolution offered by the SuperESCA beamline at ELETTRA, Trieste, allows us to study in great detail how  $C_2H_x$  adsorbates react on a Co(0001) surface, both in the absence and in the presence of CO.



Figure 1: (a) top view of C1s spectra during heating of an acetylene (+2  $H_{ad}$ )-covered Co(0001) surface in the absence (bottom) and in the presence (top) of CO (g). (b) high resolution spectra taken at the indicated temperature help to identify surface reaction intermediates (results obtained at the synchrotron in Trieste, Italy, 2018).

Ethene (CH<sub>2</sub>=CH<sub>2</sub>) adsorption at 100 K followed by heating to 220 K produces a surface covered with acetylene, HCCH + 2 H<sub>ad</sub>. Figure 1(a) shows a top view of the C1s spectral region during slow heating of this mixed layer, in vacuum (top) as well as in the presence of  $1 \times 10^{-7}$  mbar CO (bottom). In the absence of CO the acetylene adsorbate is stable up to 400 K, after which dehydrogenation produces atomic carbon. When CO is present (peaks around 285-286 eV), acetylene instead becomes reactive. The changes seen in the top view of the C1s spectra during heating shows that a first reaction occurs around 250 K, and a second reaction around 320 K.

Using high resolution photoemission spectra shown in figure 1(b) we can identify the product of the first reaction as ethylidyne (C-CH<sub>3</sub>), i.e. the presence of CO promotes acetylene hydrogenation. The product of the subsequent reaction around 320 K can be identified as 2-butyne (H<sub>3</sub>C-C=C-CH<sub>3</sub>), the product of the coupling between two ethylidyne species. Our experiments clearly show that the products of a surface

The surface reactions observed in our XPS study, C-C coupling of two adsorbed alkylidyne species and alkyne hydrogenation to alkylidyne, are important to understand the FTS chain-growth mechanism. The observed coupling of ethylidyne supports the view that FTS growth proceeds via coupling of a longchain alkylidyne with the shortest alkylidyne possible, namely the CH adsorbate. reaction are different when CO spectators are present alongside the reacting surface intermediates. This shows that factors such the nature and concentration of all adsorbates present on the surface matter and can ultimately determine which product is formed. The surface reactions observed in our study, C-C coupling of two adsorbed alkylidyne species and alkyne hydrogenation to alkylidyne, are of particular importance for the FTS chain growth mechanism. The experimentally observed propensity of ethylidyne to couple supports the view that growth under FTS conditions proceeds via the coupling of a long chain alkylidyne intermediate with the shortest alkylidyne possible, the CH adsorbate. We furthermore find that conversion of the 1-alkyne coupling product to the corresponding alkylidyne, the intermediate needed for the next CH insertion step, is promoted by CO, an adsorbate that present in high concentrations under Fischer-Tropsch synthesis conditions.

#### Thin-film iron carbide model catalysts

In the second project we aim to prepare iron carbide model catalysts by evaporation of iron into a copper (100) substrate, followed by ethylene treatments to carburize the sample. We used a combination of Auger electron spectroscopy and low energy electron diffraction to characterize the films that we prepare. After evaporating different amounts of Fe onto our Cu(100) held at room temperature we cooled the sample to 100 K and saturated the surface with ethylene. We then heated to 500 K to decompose the ethylene precursor and recorded the Auger spectrum, shown in figure 2 (left). For all iron film thicknesses we find that ethylene decomposes, and produces carbidic carbon. We furthermore find that the carbon content decreases with increasing film thickness, as shown in the figure as well (central panel). Electron diffraction reveals that the carbon causes the surface to reconstruct and we typically find a LEED pattern with a (2x2)p4g symmetry. The same pattern is found irrespective of the exact film thickness. On other (100) surfaces (e.g. Ni) the same pattern is found due to a carbon-induced reconstruction. Based on this we tentatively propose the structure shown in the figure (right). Future work will be to further characterize the FeCx films using synchrotron XPS and STM, in collaboration with Xin Yu at SynCat@Beijing. In addition to this, the chemical reactivity with CO and H2 as well as with hydrogen atoms will be explored. Finally, we currently perform similar studies using a Cu(111) crystal as a template to find out why there is such a large difference between our findings and those of Gilbère Mannie and Yijia Li (Aarhus).



Figure 2: Auger and LEED analysis after converting evaporated Fe films of different thicknesses to the carbide using ethylene as a carbon source. The shape of the carbon peak in the Auger spectrum confirms the carbidic nature of the carbon, whereas the intensity ratios of the Fe/C peaks provide information about the carbon content in the carbide. Electron diffraction gives information about the surface structure of the carbide (results obtained by Daniel Garcia at SynCat@DIFFER in 2018).

#### 5.2 Electrocatalytic processes for storing renewable energy (Dr Foteini Sapountzi)

Syngaschem investigates different electrocatalytic processes, alternative to batteries, that allow the storage of excess renewable electricity. In our applications, we use solid polymer electrolytes instead of aqueous electrolytes, because they are potentially ideally suited to intermittent supply applications at scale, offering high current densities and responsiveness to variable power input. Our activities focus on (a) hydrogen production by either water electrolysis or alcohol electrochemical reforming and (b) methanol production via CO<sub>2</sub> electroreduction.



#### Water electrolysis

This project has received funding from the EU Critcat project and Synfuels China. Our activities are focused on the specific case of polymer electrolyte membranes protonic conductivity (proton with exchange membranes, PEM). Our study addresses the main barrier to the widespread uptake of PEM water electrolyzers, that is the high capital expenditure related to the need for rare and expensive platinum group metals as electrocatalysts. Together with our collaborators, are working we on identifying alternative low-cost materials that can withstand the acidic PEM environment and also show satisfactory activity for the associated half-reactions, the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER). In general, developing a well-performing PEM electrolyzer free of noble metals is a great challenge, which has not been yet achieved. Numerous literature studies earth-abundant report alternative materials as promising catalysts for PEM water electrolysis; however these studies mainly deal with the cathodic halfreaction (HER). Finding catalysts which can be OER-active and also stable in

acidic media is still the holy grail in the field. Moreover, literature studies are still in the exploratory phase, since the majority of them focuses on model catalysts (typically glassy-carbon) operated under simulated environment (batch electrochemical cells with aqueous electrolytes). Less than 1% of the reported studies have actually tested earth-abundant catalysts under realistic PEM water electrolysis conditions. In such systems, 3D catalysts (gas diffusion electrodes) are interfaced to polymeric membranes and are employed in real flow-through PEM water electrolysers. Thus, our activities position us in the very few groups worldwide who have attempted to work on the actual challenge of introducing earth-abundant materials into Membrane Electrode Assemblies (MEAs) and testing them in real PEM electrolysis units such as the one shown in Figure 3a.

Our efforts have been focused on using transition metal sulfides (such as  $MoS_2$ ) and phosphides (such as  $NiP_2$ ) and optimizing the electrode design of the HER electrode (cathode) and OER electrode (anode). Overall, our results so far are not very encouraging regarding full replacement of PEM electrolysers electrodes with PGM-free catalysts, since all the materials we tested showed poor performance for OER.

However, this is not the case for the cathode. Our results till now show that half-replacement of PEM electrolyzer materials by alternative more abundant materials is feasible.

In collaboration with the Iberian National Laboratory (INL), the Iowa State University and the U.S. Department of Energy, two polymorphs of NiP<sub>2</sub> were synthetized, characterized and tested as HER electrocatalysts in a PEM electrolyzer. Our investigations demonstrated that the electrocatalytic performance is very sensitive to the peculiar features of the crystal structures, with *cubic-NiP<sub>2</sub>* outperforming *monoclinic-NiP<sub>2</sub>*. The required potentials to reach current densities of 100 mA/cm<sup>2</sup> when using a *c-NiP<sub>2</sub>*/Nafion/ IrRuO<sub>x</sub> assembly are only 12-15 % higher compared to the state-of-the-art Pt/Nafion/IrRuO<sub>x</sub> assembly. Even though NiP<sub>2</sub> does not outperform Pt in PEM electrolysis, its moderate HER activity can be of practical importance due to its significantly lower cost and thus *c-NiP<sub>2</sub>* can be considered as a promising alternative cathode for PEM electrolyzers. The durability of *c-NiP<sub>2</sub>* was confirmed under 48-h continuous operation. This work has already been submitted for publication. Further research on this topic is planned for 2019 to fabricate NiP<sub>2</sub>-based MEAs with improved activity and also to potentially use other materials as electrocatalysts (such as FeP or Ni<sub>3</sub>B).



Figure 3, left: Schematic of the PEM electrolysis setup where hydrogen is produced via electrolysis of water vapors; right: Polarization curves with  $IrRuO_x$  anode, Nafion membrane electrolyte and cathodes of m-NiP<sub>2</sub>, c-NiP<sub>2</sub> (2 mg/cm<sup>2</sup>) and Pt (0.5 mg/cm<sup>2</sup>)

Another part of our activities concerns the use of  $MoS_2$  as an alternative HER electrocatalyst. We are working together with the National Physics Laboratory of UK and the Eindhoven University of Technology in order to configure an electrode design with optimized catalyst utilization. For this reason, we use  $MoS_2$  deposited by various techniques (Atomic Layer Deposition, Electrodeposition, Ink spray deposition) on different porous supports (carbon paper or cloth, Inconel etc). Preliminary results have been obtained and this research is planned to be completed within 2019.

#### Hydrogen at low potential from electrochemical reforming of alcohols

Alcohol electrolysis or electrochemical reforming of alcohols allows hydrogen production at lower potentials (~0.1 V) compared to the conventional water electrolysis (1.23 V). Hydrogen evolution takes place at the cathode, and alcohol electrooxidation at the anode, replacing the sluggish oxygen evolution of the

conventional water electrolyzers. Even though  $CO_2$  is also produced, the overall process can be green if the alcohol originates from biosources. The concept is not only limited to the use of alcohols, since several other organic compounds have been also successfully used in literature. This approach is a promising alternative to the conventional water electrolysis and it has received much attention lately (figure 4).

Alcohol electrolysis can be realized with solid polymer electrolytes with either  $H^+$  (acidic) or  $OH^-$  (alkaline) conductivity, but each approach has its own pros and cons. As shown in figure 5, when using a  $H^+$  conductor, pure  $H_2$  is produced only at the cathode (separated by other reaction products or reactants), while this is not the case for  $OH^-$  conductors. On the other hand, it is well established in literature that the anodic half-reaction (alcohol electro-oxidation) is highly pH-sensitive and very much favored in alkaline media. We have been the first to compare and analyze the performance of acidic and alkaline alcohol electrolysers operating under identical conditions.

Syngaschem and DIFFER are working actively in the field of alcohol electrolysis since 2015 (with funding from Synfuels China and EU Critcat project), while theInstitute of Polymers of the Bulgarian Academy of Sciences (IP-BAS) was also introduced in this consortium in 2016. Within 2018 our results have been communicated as oral presentations in 2 international events (69<sup>th</sup> Annual Meeting of the International Society of Electrochemistry, International Symposium on Electrocatalysis). An article has been submitted for publication in the International Journal of Hydrogen Energy (accepted in March 2019).



Figure 4 Number of publications dealing with the concept of water electrolysis assisted by organic compounds (mainly alcohols) over the last decade. Red stars correspond to articles (co-)authored by F. Sapountzi.

In general, till now it has been found that alkaline ethanol electrolysis can perform better than the acidic, provided that appropriate reaction conditions are applied related to the exact composition of the anolyte solution. However, even though the process is kinetically favored in the alkaline environment, there are several features related with the polymeric membrane that also affect significantly the overall performance, such as the extent of ethanol crossover through the membrane, the ionic conductivity and the swelling behavior in presence of ethanol.

Since the necessity of optimizing several properties of the membrane has become clear, IP-BAS has already synthetized several chemically linked alkaline membranes with appropriate modifications in order to address the issues of chemical stability and conductivity. Our plan for 2019 is to continue our studies using the newly developed membranes, aiming to further enhance the performance of alcohol electrolyzers.



Figure 5 Operation principle of acidic and alkaline methanol electrolysis.

#### Electrochemical reduction of CO<sub>2</sub>

In the frame of the Critcat project, we work jointly with DIFFER on the development of compact reactors that can selectively convert  $CO_2$  into methanol or CO.  $CO_2$ -electroreduction has been intensively studied in literature using model catalysts in aqueous electrolyte solutions. In general, this reaction has a broad product distribution, while both selectivity and activity are greatly affected by the nature of the electrocatalyst, its structural characteristics, the pH, the exact composition and nature of the electrolyte solution. Apart from tuning the C-selectivity towards a desired product, another great challenge related with this reaction is the need to suppress the competing hydrogen evolution reaction.

Using porous electrocatalysts based on titania nanotubes and  $OH^-$  conducting polymer membrane electrolytes, we managed to reach 100% C-selectivity to methanol but our current systems exhibit overall selectivity to  $CO_2$  electroreduction of 20%, with the rest 80% accounting for the competing hydrogen evolution. Our plan in 2019 is to further promote C-selectivity by properly tuning the structure of the titania nanotubes.



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

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

#### Micro reactor for testing powders and flat model catalyst models

The in-house developed micro reactor with in-situ UV-vis spectroscopy (see figure) that has previously been used for characterization of both flat model catalysts and powder catalysts in reactions like H<sub>2</sub>, and CO oxidation as well as water gas shift reaction has been further improved. During 2018, it has been used to test various catalysts for NH<sub>3</sub> decomposition, combustion of volatile organic compounds (VOC) and preferential oxidation of CO in hydrogen (PROX). For flat model catalysts, UV-vis spectroscopy has been used to monitor changes in the oxidation state during use.



Figure 6 The micro reactor with in-situ UV-vis and mass spectroscopy has played an important part in testing various catalysts, both of flat model and powder type. It combines high sensitivity with rapid accomodation to changinges in temperature and composition of the reacting gases, and enables instantaneous oxidation state analysis of the catalysts via UV-Vis spectroscopy.

#### Model catalysts for FTS, NH<sub>3</sub> decomposition and combustion of volatile organics

A wide range of catalysts has been tested for the ammonia decomposition reaction. The aim was to find an efficient catalyst that uses a minimum of Ru, the catalyst that is currently the most active. An NH<sub>3</sub>- decomposition catalyst can find application for cleaning up gas streams or for liberating H<sub>2</sub> if NH<sub>3</sub> has been used for storing of H<sub>2</sub>. Both mono and bimetallic catalyst have been tested. Powder catalyts prepared via conventional impregnation of alumina supports have been used for reference. Mono disperse, Ru, Ru-Ni and Ru-Co colloids have then been prepared and impregnated onto the alumina supports. The final set of samples were flat model catalysts, where Ru, Ru-Co, Fe-Co and Fe were produced by supersonic cluster deposition techniques and deposited onto quartz wafers. The activity towards ammonia decomposition for all these catalysts is shown in the figure. In conclusion, no catalyst was found to challenge the activity of pure Ru-catalyst. In fact, adding a second metal generally decreased the activity of the catalyst, most likely due to blocking of the active surface. Nickel is the only catalyst that may challenge Ru, not on a weight basis



Figure 7 NH<sub>3</sub> decomposition as a function of temperature on bi-metallic Ru-Co powder catalysts (left) and flat model catalysts of Ru, Ru-Co, Fe-Co and Fe (right).

but on a cost basis, since Ni is so much cheaper than Ru. The research was done together with the CritCat groups from Italy, Germany, Portugal, and with UCT South Africa, and is being prepared for joint publication.

#### 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 active, even without inclusion of Pt. These results are presently being written up for a publication. The research was conducted in collaboration with groups from Italy, Germany and Portugal in the CritCat project.

#### Model catalysts by Atomic Layer Deposition and cluster deposition

The range of flat model catalyst that has been used in the micro reactor has been extended beyond evaporated thin films and powders to include size selected nanoclusters from Pt, Ni-Pt and Cu-Pt and Co nanoparticles prepared by atomic layer deposition (ALD). The former has been tested for hydrogen oxidation and VOC-combustion while the latter has been tested for NH<sub>3</sub> decomposition and CO methanation. This work, in collaboration with the CritCat groups from Italy, Germany and Netherlands will be continued during 2019. Additional approaches for flat model catalyst preparations will be evaluated.

### 6. International Collaborations

#### 6.1 MagnetoCat SLU, Alicante Spain (Dr Jose Gracia)

Since Dr Gracia left SynCat@Beijing and Syngaschem BV to start his own research enterprise MagnetoCat, we have fruitfully collaborated on several projects, in electrochemistry (oxygen evolution reaction in perovskites) and in Fischer-Tropsch catalysis. In 2018, a study on the structures of iron and iron carbide monolayer structures on copper substrates became complete, which compares well with the experiments of PhD student Daniel Garcia (as discussed in Figure 2 herefore). A joint publication is foreseen in 2019. Together with a PhD student from the University of Zaragoza, Jose Gracia made a mechanistic study of the Fischer-Tropsch reaction on iron carbides, which fully incorporates magnetic properties of the catalyst.

#### 6.2 Collaboration with the University of the Free State, Bloemfontein

Prof dr Jannie Swarts, Dr Blener Buitendach, Dr Lizette Erasmus, Dr Ernie Langner



Under direction of Prof J.C. Swarts, Dr Buitendach has performed very interesting research on the synthesis and characterization of Mn-Fe<sub>n</sub> and Ir-Ru multinuclear clusters, in a project that has been sponsored by Syngaschem BV for several years. Our interest is to use these elegant complexes as precursors for precision



catalysts on the model scale. The work has so far led to 3 publications on the synthesis, characterization and molecular properties of the Mn-Fe complexes in Inorganic Chemistry (2x; see the graphical abstracts above), and on detailed photoemission studies in Molecules. In 2018, Blener Buitendach has worked on bi- and multinuclear Ir-Ru complexes, as precursors for oxygen evolution catalysts. In May he visited the SynCat@DIFFER lab for several weeks to collaborate with Foteini Sapountzi.



Dr Lizette Erasmus works on a project aimed at  $CO_2$  capture by Frustrated Lewis Pairs. These are complexes of acids and bases in which steric constraints prevent them to form close bonds. As a result they leave space and 'open charges' where  $CO_2$  can bind and possibly also react. Dr Erasmus' plans are to anchor such complexes to a support, either both or one of the components, and investigate them for  $CO_2$  capture / release, and for reaction, e.g. to formic acid.



In another approach to  $CO_2$  capture, Dr Ernie Langner uses metal organic frameworks of the Zeolitic Imidazolic Framework type, ZIF-8. By sensitizing the ZIF by means of solvent-assisted ligand exchange, he could enhance the already appreciable  $CO_2$ sorption capacity of ZIF-8 by another 67% by using the compound 2-nitro imidazole. This successful work was published in Microporous and Mesoporous Materials. The work has been extended by molecular modeling to obtain leads for further improvement of the metal organic frameworks for  $CO_2$  capture, storage and release.

On November 19, 2018 a workshop was held in Bloemfontein to discuss progress and further plans for 2019.

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#### 6.3 University of Cape Town, c\*change program

Prof dr Michael Claeys, Dr Nico Fischer, Rosalind Stegmann, Muhamed Fadlala



Syngaschem BV also sponsors collaborative projects in the Research Group of Prof Michael Claeys and Dr Nico Fischer at the University of Cape Town, 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. The figure above shows a scheme of their famous in situ magnetic analysis equipment, along with measurements on two iron catalysts (pure iron in blue, promoted iron in red) during Fischer-Tropsch synthesis, while progressively more water is added into the reactor (project of Ms Rosalind Stegmann). The increase in magnetization in the upper panel is caused by the oxidation of the - at this reaction temperature - paramagnetic iron carbide  $Fe_5C_2$  into the ferromagnetic iron oxide  $Fe_3O_4$ .



Dr Muhamed Fadlala carries out highly detailed research on the product distributions of Fischer-Tropsch synthesis by using a two-dimensional gas chromatography technique GCxGC. The figure left shows examples of Fischer-Tropsch synthesis at three temperatures on a cobalt catalyst. The 2D-GC or GCxGC patterns indicate the presence of hydrocarbons (mostly paraffins, and some olefins) while more complicated products such as aromatics and oxygenates are virtually absent from the product distribution. This is of interest in view of recent claims in the literature that cobalt and cobalt carbide catalysts could be used for olefin and alcohol selective Fischer-Tropsch synthesis.

Finally, Dr Nico Fischer has helped us with the synthesis and characterization of a range of standard catalysts, which have played an important role in the ammonia decomposition research described earlier in this report. The projects with the University of Cape Town will all be continued in 2019.

We are very pleased that Prof Michael Claeys has agreed to serve as official advisor of Syngaschem BV.





## 7. Collaboration and interaction with SynCat@Beijing

Frequent interaction exists between the two SynCat laboratories, and several joint publications appeared, in the area of mechanistic Fischer-Tropsch research, and on electrolysis of water. Due to illness, Hans Niemantsverdriet could not make any visits to Beijing in 2018. Owing to weekly reports by the staff he could nevertheless follow the activities.

Kees-Jan Weststrate visited SynCat@Beijing three times:

- *February 4-February 9: for meetings* with SynCat staff in surface science, and to work on an update of the TPD equipment.
- April 13-April 21: to participate in "Workshop at SynCat@Beijing" (April 17-18), consisting of a visit by and presentations from all researchers working in the SynCat@DIFFER program in Eindhoven, and to have meetings with SynCat surface science staff, and work on the manipulator of the TPD setup at Beijing.
- September 17-September 22: Invited talk at Institute of Coal Chemistry, "Taiyuan Energy Low Carbon Development Forum", meetings with SynCat surface science staff, and for installation and testing of the TPD manipulator at SynCat@Beijing.

Jan-Karel Felderhof visited SynCat@Beijing for a week from March 24 – 31 to present a short lecture on leadership development, and to hold individual coaching meetings with all SynCat staff members.

Hans Fredriksson visited SynCat@Beijing from *April 13-April 21 to participate in* "Workshop at SynCat@Beijing" (April 17-18), and to have meetings with SynCat staff.

The SynCat-DIFFER workshop featured prominently on the front page of the Synfuels China Monthly Journal of May 2018 (see adjacent page).



Left: Prof. Yongwang Li opens the SynCat-DIFFER workshop with an introduction to Synfuels China and Coal-to-Liquids technology. Right: Dr. Kees-Jan Westrate presents the research program of SynCat@DIFFER. Besides SynCat@Beijing staff and DIFFER Guests, the workshop also attracted researchers from the Synfuels China research laboratories; all-in alla bout 30 participants attended. (*Photos by Ajin Cheruvathur*).





#### 中科合成油技术有限公司综合部主办

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## 1<sup>st</sup> SynCat-DIFFER worksop was held at SynCat@Beijing on Apr 17<sup>th</sup>-18<sup>th</sup>



Report&Photos by Ajin Cheruvathur.

As the part of enhancing the scientific contaboration between SynCat@Beijing and Ducth Institute of Fundamental Energy Research (DIFFER), Eindhoven; a group of researchers from DIFFER visitedSynCat@Beijing on 16th - 18th April 2018. Dr. Kees-Jan Westrate, the deputy director of Syngaschem (SynCat@DIFFER) led the group of three post-docs, two PhD students and a senior research scientist. On 16th, the group visited the different labs in SynCat and discussed with the SynCat researchers about the possibilities of utilising the research facilities in SynCat as a complimentary research tool for their ongoing research at DIFFER. On 17th and 18th a workshop was held at Einstein room, SynCat; where all SynCat staff as well as the guests from DIFFER. presented theirr esearch progress.

On 17th, the workshop stared with an introductory lecture by Prof. Yongwang Li on the differences in the research methodologies in different countries and importance of international collaborations and research in a different lab to absorb the positive sides of the other methodology to improve the existing methodology.Next,Dr.Kees-JanWestrateintroduced the Chemical Industrial Partnership Program (CHIPP), which provides the subsidy for this visit and to do research in collaboration with industry. He also gave an overview of the surface science research programs in DIFFER. The lectures in the second session of the workshop was about the iron based Fischer Tropsch catalysts and in-situ characterization techniques for the model catalysis studies. Dr. Xi Liu from SynCat, delivered the first lecture about the latest developments in the in-situ TEM with the in-situ TEM on the soot-oxidation over Ag-CeO, as an example. Later, Dr. Xin Yu from SynCat gave a lecture on the surface chemistry and morphology of iron oxide on Ru, Pt and Cu single crystal under CO, CO, and / or H2 atmosphere. The next talk was from Mr. Daniel Rodiguez(DIFFER); which is about the Feevaporation and the resulted superstructures over Cu single crystal, After lunch, Dr. Gilbère Mannie talked about the formation of iron oxide/iron carbide times on Au and Cu single crystals as the model system for Iron basedFTcatalyst.Subsequently,Dr.HansFredriksson (senior scientist from SynCat@DIFFER) described the fabrication and testing of various flat and 3D model catalysts for Fischer-Tropsch, reverse water gas shift reaction and soot oxidation. The last lecture in the session was from Dr. Ling Zhang from SynCat. She presented the syngas conversion over Fe and Cr based perovskite catalysts (with or without Zeolites) towards the selective production of olefins. The only presentation in the third session (new concepts in catalysis) was from Dr. Qin Ong (DIFFER). Her talk was about the about the application of plasma for the vibrational activation surface interaction. She showedCO, reduction to COas a model reaction with a plasma activated CO, as the reactant. After conclusion of first day lectures, SynCat researchers and guests from DIFFER joined for the dinner at CFGC grand hotel, where they continue the scientific discussion.

The first lecture of the second day of workshop and the first lecture of electro catalysis and perovskite materials session was delivered by Dr. Vasilis Kyriakou (DIFFER). His topic of presentation was about the Co-electrolysis of H<sub>2</sub>O-CO<sub>3</sub> towards syngas in solid oxide fuel cells. After that, Dr Tingbin Lim (SynCat) explained how the spin of the transition metal in a perovskite catalyst can influence the oxygen evolution and oxygen reduction reactions. The synthesis of perovskites based on this DFT-design

principles, and performance of these perovskites as OER/ORR and de-NOx catalyst was the topic of next talk; which was given by Dr. Ajin Cheruvathur from SynCat. The fifth session of the workshop was about the cobalt based Fischer-Tropsch synthesis. The first talkwasgivenbyDr.TianfuZhangfromSynCat;which was about the CO hydrogenation over cobalt carbide, studied under UHV and industrial conditions. The next talk in the session was from Dr. Gerben van Straaten from DIFFER. He demonstrated the preparation of Co model catalysts by vapour deposition methods. After the junch, Mis. Devyam Sharma from DIFFER talked about differences in the CO and hydrogen adsorption behaviour on Flat, stepped and kinked Cosingle crystal surfaces. The last talk in the session was delivered by Dr. Xiong Zhou. His lecture was about probing the iron carburization over Fe thin films over Si single crystal with silica layer by means of in-situ NAP-XPS. The only talk in the last session (photocatalysis) of the workshop was given by Dr. Ren Su which was about the photocatalytic organic synthesis in the wide range, from fundamental reaction mechanistic studies in UHV system to the large scale synthesis using sunlight.

The workshop initiated lot of discussion on the potential collaborations between SynCatand DIFFER researchers. Hopefully, in future some collaboration projects will happen in a way to utilize the research facilities in the SynCat for the DIFFER researchers and viceversa.



DI. Received we workshop also attracted researchers other than SynCat staff as well as guests from DIFFER leads to more than 30 participants.

The SynCat-DIFFER Workshop featured prominently on the front page of the Synfuels China Monthly of May 2018

## 8. Publications and Conference Appearances 2018

#### 8. 1 Core Publications of Syngaschem BV

- **1.** CO as a Promoting Spectator Species of C<sub>x</sub>H<sub>y</sub> Conversions Relevant for Fischer-Tropsch Chain Growth on Cobalt: Evidence from Temperature-Programmed Reaction and Reflection Absorption Infrared Spectroscopy; Weststrate, C.J.; Niemantsverdriet, J.W.; ACS CATALYSIS 8 (2018) 10826-10835
- Preferential oxidation of CO in H<sub>2</sub> on Cu and Cu/CeO<sub>x</sub> catalysts studied by in situ UV-Vis and mass spectrometry and DFT; Bu, Yibin; Er, Suleyman; Niemantsverdriet, J.W.; Fredriksson, Hans O.A.; JOURNAL OF CATALYSIS 357 (2018) 176-187
- **3.** Application of work function measurements in the study of surface catalytic reactions on Rh(100) Caglar, Basar; Kizilkaya, Ali Can; Niemantsverdriet, J.W. (Hans); Weststrate, C.J. (Kees-Jan) CATALYSIS STRUCTURE & REACTIVITY 4 (2018) 1-11
- 4. Can Electrochemical Measurements Be Used To Predict X-ray Photoelectron Spectroscopic Data? The Case of Ferrocenyl-beta-Diketonato Complexes of Manganese(III) Buitendach, Blener E.; Erasmus, Elizabeth; Niemantsverdriet, J.W. (Hans); Swarts, Jannie C. INORGANIC CHEMISTRY 57 (2018) 6606-6616
- 5. Enhanced CO<sub>2</sub> adsorption in nano-ZIF-8 modified by solvent assisted ligand exchange Tsai, Chih-Wei; Niemantsverdriet, J.W. (Hans); Langner, Ernie H. G.; MICROPOROUS AND MESOPOROUS MATERIALS 262 (2018) 98-105

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

- 6. Relationship between Iron Carbide Phases (epsilon-Fe<sub>2</sub>C, Fe<sub>7</sub>C<sub>3</sub>, and chi-Fe<sub>5</sub>C<sub>2</sub>) and Catalytic Performances of Fe/SiO<sub>2</sub> Fischer-Tropsch Catalysts; Chang, Qiang; Zhang, Chenghua; Liu, Chengwei; Wei, Yuxue; Cheruvathur, Ajin V.; Dugulan, A. Iulian; Niemantsverdriet, J. W.; Liu, Xingwu; He, Yurong; Qing, Ming; Zheng, Lirong; Yun, Yifeng; Yang, Yong; Li, Yongwang; ACS CATALYSIS 8 (2018) 3304-3316
- 7. Iron Carbidization on Thin-Film Silica and Silicon: A Near-Ambient-Pressure X-ray Photoelectron Spectroscopy and Scanning Tunneling Microscopy Study; Zhou, Xiong; Mannie, Gilbere J. A.; Yin, Junqing; Yu, Xin; Weststrate, C. J.; Wen, Xiaodong; Wu, Kai; Yang, Yong; Li, Yongwang; Niemantsverdriet, J. W.; ACS CATALYSIS 8 (2018) 7326-7333
- 8. Efficient Solar-Driven Hydrogen Transfer by Bismuth-Based Photocatalyst with Engineered Basic Sites; Dai, Yitao; Li, Chao; Shen, Yanbin; Zhu, Shujie; Hvid, Mathias S.; Wu, Lai-Chin; Skibsted, Jurgen; Li, Yongwang; Niemantsverdriet, J. W. (Hans); Besenbacher, Flemming; Lock, Nina; Su, Ren; JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 140 (2018) 16711-16719
- 9. In-situ probing photocatalytic C-C bond cleavage in ethylene glycol under ambient conditions and the effect of metal cocatalyst; Li, Chao; Wang, Xiaoping; Cheruvathur, Ajin; Shen, Yanbin; Xiang, Hongwei; Li, Yongwang; Niemantsverdriet, J. W.; Su, Ren; JOURNAL OF CATALYSIS 365 (2018) 313-319
- 10. Intercalation Mechanisms of Fe Atoms underneath A Graphene Monolayer on Ru(0001) Zhao, Peng; Ren, Pengju; Weststrate, C. J. Kees-Jan; Xu, Yuqun; Cao, Dong-Bo; Xiang, Hongwei; Xu, Jian; Yang, Yong; Li, Yong-Wang; Niemantsverdriet, J. W. (Hans); Wen, Xiaodong; Yu, Xin JOURNAL OF PHYSICAL CHEMISTRY C 122 (2018) 22903-22910
- 11. Orbital Physics of Perovskites for the Oxygen Evolution Reaction; Sharpe, Ryan; Munarriz, Julen; Lim, Tingbin; Jiao, Yunzhe; Niemantsverdriet, J.W.; Polo, Victor; Gracia, Jose; TOPICS IN CATALYSIS 61 (2018) 267-275
- **12.** Principles determining the activity of magnetic oxides for electron transfer reactions; Gracia, Jose; Sharpe, Ryan; Munarriz, Julen; JOURNAL OF CATALYSIS 361 (2018) 331-318

#### 8.3 Publications under submission

- Overpotential analysis of alkaline and acidic alcohol electrolysers and optimized membrane-electrode assemblies, Sapountzi, F.; Di Palma, V; Zafeiropoulos, G.; Penchev, H.; Verheijen, M.A.; Creatore, M.; Ublekov, F.; Sinigersky, V.; Fredriksson, H.O.A.; Tsampas, M.N.; Niemantsverdriet, J.W.; INTERNATIONAL JOURNAL OF HYDROGEN TECHNOLOGY 2019 (accepted)
- 2) Effect of Ammonia on Cobalt Fischer-Tropsch Synthesis Catalysts: A Surface Science Approach, Kizilkaya, A.C.; Niemantsverdriet, J.W.; Weststrate, C.J.; CATALYSIS SCIENCE AND TECHNOLOGY 2019 (accepted).
- 3) Solid Base Bi<sub>24</sub>O<sub>31</sub>Br<sub>10</sub>(OH)<sub>δ</sub> with Active Lattice Oxygen for Efficient Photo-oxidation of Primary Alcohols to Aldehydes, Dai, Y.; Ren, P.; Li, Y.; Lu, D.; Shen, Y.; Li, Y.W.; Niemantsverdriet, J.W.; Besenbacher, F.; Xiang, H.; Hao, W.; Lock, N.; Wen, X.; Lewis, J.P.; Su, R.; ANGEWANDTE CHEMIE 2019 (accepted).
- 4) Atomically Defined Iron Carbide Surface for Fischer–Tropsch Synthesis Catalysis, Li, Y.; Li, Z.; Ahsen, A.; Lammich, L.; Mannie, G.J.A.; Niemantsverdriet, J.W.; Lauritsen; J.V.; ACS CATALYSIS 2019 (accepted).
- 5) NiP<sub>2</sub>: A story of two divergent polymorphic catalysts, Owens-Baird, B.; Xu, J.; Petrovykh, D.; Bondarchuk, O.; Ziouani, Y.; Gonzalez-Ballesteros, N.; Yox, P.; Sapountzi, F.M.; Niemantsverdriet, J.W.; Kolen'ko, Y.V.; Kovnir, K.; CHEMISTRY OF MATERIALS (submitted)

#### 8.4 Oral Contributions at Conferences

- 1. <u>C.J. Weststrate</u>, J.W. Niemantsverdriet, "CO As an Active Spectator Species in Hydrocarbon Conversions Related to Fischer-Tropsch Synthesis", Netherlands' Catalysis and Chemistry Conference XIX, March 7, Noordwijkerhout, Netherlands
- <u>A.C. Kizilkaya</u>, J.W. Niemantsverdriet, C.J. Weststrate "A molecular perspective on the poisoning of cobalt Fischer-Tropsch Synthesis catalysts by ammonia", Netherlands' Catalysis and Chemistry Conference XIX, March 7, Noordwijkerhout, Netherlands
- 3. "Research on Catalysis for Storing Renewable Electricity", H. O. A. Fredriksson, 9th European Networking Event: Successful R&I in Europe, Dusseldorf, D, 15-16 March, 2018
- 4. <u>C.J. Weststrate</u>, D. Sharma, D. Garcia Rodriguez, J.W. Niemantsverdriet, "Shapes and Sites, Coverages and Mechanisms: FTS through the Eyes of a Surface Chemist", SynGas Convention 3, 27 March, Cape Town, South-Africa
- 5. <u>A.C. Kizilkaya</u>, J.W. Niemantsverdriet, C.J. Weststrate "A molecular perspective on the poisoning of cobalt Fischer-Tropsch Synthesis catalysts by ammonia", SynGas Convention 3, 27 March, Cape Town, South-Africa
- <u>F. Sapountzi</u>, V. Di Palma, G. Zafeiropoulos, H. Penchev, M.A. Verheijen, M. Creatore, F. Ublekov, V. Sinigersky, H.O.A. Fredriksson, M.N. Tsampas, J.W. Niemantsverdriet, "Analysis of acidic and alkaline alcohol electrolysis and development of novel membrane-electrode assemblies", International Symposium on Electrocatalysis, August 29- September 1, Szczyrk, Poland
- 7. <u>H.O.A. Fredriksson</u>, "In situ UV-vis Characterization & Activity Testing of Flat Model Catalysts in Custom Built Micro Reactors", 34th Eur. Conference on Surface Science (ECOSS 34), Aarhus, Dk, 26-31 Aug. 2018
- 8. <u>C.J. Weststrate</u>, J.W. Niemantsverdriet, "CO As an Active Spectator Species in Hydrocarbon Conversions Related to Fischer-Tropsch Synthesis", Eur. conference on Surface Science, 29 August, Aarhus, Denmark
- 9. <u>D. Garcia Rodriguez</u>, D. Sharma, J.W. Niemantsverdriet, C.J. Weststrate, "Preparation of single crystalline iron carbide model catalysts for syngas conversion via the Fischer-Tropsch synthesis", European conference on Surface Science XXXIV, 29 August, Aarhus, Denmark
- 10. M.D. Strømsheim, I.-H. Svenum, M. H. Farstad, C.J. Weststrate, A. Borg, H. Venvik Johnsen
- 11. "The CO-induced surface reconstruction on Co(11-20)— a combined theoretical and experimental investigation", European conference on Surface Science XXXIV, 29 August, Aarhus, Denmark

- 12. <u>F. Sapountzi</u>, V. Di Palma, G. Zafeiropoulos, H. Penchev, M.A. Verheijen, M. Creatore, F. Ublekov, V. Sinigersky, H.O.A. Fredriksson, M.N. Tsampas, J.W. Niemantsverdriet, "Material considerations for making alcohol electrolysis more efficient: Acidic vs alkaline polymer electrolytes and novel anode architectures", 69<sup>th</sup> Annual Meeting Intern. Society of Electrochemistry, September 2-7, Bologna, Italy
- 13. <u>H.O.A. Fredriksson</u>, "In situ studies of model catalysts for heterogeneous catalysis", 2nd Global Conference on Catalysis, Chemical Engineering & Technology, (CAT 2018), Sept. 13-15, 2018, Rome, Italy
- Invited, <u>C.J. Weststrate</u>, J.W. Niemantsverdriet "Surface Science investigations of the Fischer-Tropsch Reaction on Cobalt and Iron Model Catalysts", Taiyuan Energy Low Carbon Development Forum, 17 September 2018, Institute of Coal Chemistry, Taiyuan, P.R. China

#### 8.5 Contributions at Conferences (posters)

- F. Sapountzi, V. Di Palma, G. Zafeiropoulos, H. Penchev, M.A. Verheijen, M. Creatore, F. Ublekov, V. Sinigersky, H.O.A. Fredriksson, M.N. Tsampas, J.W. Niemantsverdriet, "Hydrogen production via electrochemical reforming of alcohols", Netherlands' Catalysis and Chemistry Conference XIX, March 7, Noordwijkerhout, Netherlands
- <u>G. Zafeiropoulos</u>, J. Zhou, F.M. Sapountzi, J.W. Niemantsverdriet, T. Stoll, M.N. Tsampas, "CO<sub>2</sub> fixation in a novel (photo)electrochemical cell", Netherlands' Catalysis and Chemistry Conference XIX, March 7, Noordwijkerhout, Netherlands
- 3) <u>D. García Rodríguez</u>, D. Sharma, C.J Weststrate, J.W. Niemantsverdriet, "Fe evaporation on Cu(100) for iron carbide model catalysts for syngas conversion for FTS", Netherlands' Catalysis and Chemistry Conference XIX, March 7, Noordwijkerhout, Netherlands
- 4) <u>D. Sharma</u>, D. García Rodríguez, C.J Weststrate, J.W. Niemantsverdriet, "", Netherlands' Catalysis and Chemistry Conference XIX, March 7, Noordwijkerhout, Netherlands
- 5) R. Stegmann, N. Fischer, H. Kotze, H. Niemantsverdriet, M. Claeys, Oxidation and re-carburization of iron-based catalysts captured in-situ, SynGas Convention 3, 25 March, Cape Town, South-Africa
- 6) <u>M.I. Fadlala</u>, J.W. Niemantsverdriet, N. Fischer, M. Claeys, Influence of potassium promotion in nickel ferrite for total and specific oxygenates formation in Fischer-Tropsch; 2D-GC study, SynGas Convention 3, 25 March, Cape Town, South-Africa
- 7) <u>D. Sharma</u>, D. García Rodríguez, J.W. Niemantsverdriet, C.J Weststrate, "CO adsorption and dissociation on flat, stepped and kinked Co surface", European conference on Surface Science XXXIV, 29 August, Aarhus, Denmark
- <u>R. Stegmann</u>, N. Fischer, H. Kotzé, H. Niemantsverdriet' M. Claeys, Oxidation and re-carburization of Febased Fischer-Tropsch synthesis catalysts captured in-situ, 29<sup>th</sup> Annual CATSA Conference, 11 - 14 November 2018, Limpopo,
- 9) <u>M.I. Fadlala</u>, N. Fischer, J.W. Niemantsverdriet, M. Claeys, Beyond olefins and paraffins detailed analysis of Fe-based FTS as function of temperature: 2D GC study, 29<sup>th</sup> Annual CATSA Conference, 11 - 14 November 2018, Limpopo

#### 8.6 Seminars at Institutes and Universities

- 1) <u>C.J. Weststrate</u>, "Fundamental insights into the Fischer-Tropsch synthesis reaction on Cobalt: taking the surface science approach", SynCat@Beijing, 8 February 2018, Huairou
- 2) <u>C.J. Weststrate</u>, "Shapes and Sites, Coverages and Mechanisms: FTS through the Eyes of a Surface Chemist", SynCat workshop, 17 April 2018, Huairou, P.R. China
- 3) <u>H.O.A. Fredriksson</u>, F.M. Sapountzi, CritCat Progress Meeting (Month 24) "WP4 Model catalyst preparation and testing," 18 June 2018, Trondheim, Norway
- 4) <u>H.O.A. Fredriksson</u>, F.M. Sapountzi, CritCat Progress Meeting (Month 24) "WP5 Catalyst development and optimization", 18 June 2018, Trondheim, Norway

- 5) <u>C.J. Weststrate</u>, "Preparation of single crystalline iron carbide model catalysts for syngas conversion via the Fischer-Tropsch synthesis", SynCat@Beijing, 21 September 2018, Huairou
- 6) <u>F.M. Sapountzi</u>, "Basic electrocatalysis", Syngaschem-Fontys Science meeting, 27 September 2018, Eindhoven, Netherlands
- 7) <u>H.O.A. Fredriksson</u>, F.M. Sapountzi, CritCat Progress Meeting (Month 30) "WP4 Model catalyst preparation and testing", 30-31 October 2018, Swansea, UK
- 8) <u>H.O.A. Fredriksson</u>, F.M. Sapountzi, CritCat Progress Meeting (Month 30) "WP5 Catalyst development and optimization", 30-31 October 2018, Swansea, UK
- 9) <u>F.M. Sapountzi</u>, "Material considerations for making alcohol electrolysis more efficient", Solar fuels Science meeting, DIFFER, 29 October 2018, Eindhoven, Netherlands
- 10) J.W. Niemantsverdriet, Research at Syngaschem BV, Workshop on Syngaschem-sponsored research at the University of Cape Town, 16 November 2018, Cape Town, South Africa
- 11) J.W. Niemantsverdriet, Research at Syngaschem BV, Workshop on Syngaschem-sponsored projects at the University of the Free State, 19 November 2018, Bloemfontein, South Africa

## 9. Sponsorships in 2018

At the occasion of its fifth anniversary, Syngaschem BV has sponsored the 3<sup>rd</sup> Syngas Convention, Cape Town, March 2018, and also the Dutch Chemistry Conference ""CHAINS" Veldhoven, December 2018. In May 2018, it also supported the National Sports Contest of the Dutch Chemistry Students. ONCS 2018. In conferences sponsored by Syngaschem, the following advertisement was published in the program book.

On a regular basis, 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 occasion, it sponsors local cultural events, such as the Mierlo Jazz Festival of the JazzCape Big Band, July 7, 2018.



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In 2013, Yong-Wang Li, Synfuels China Technology, and Hans Niemantsverdriet, TU Eindhoven decided to build a new international laboratory for fundamental research, SynCat@Beijing, with a branch in Eindhoven. Syngaschem BV was established as Dutch SME to support recruitment of staff and buy instrumentation. Now it runs a small laboratory entitled SynCat@DIFFER, at the Dutch Institute for Fundamental Research, with projects on syngas, and electrolysis.

Five years after the start, the two SynCat laboratories are in full swing. Syngaschem's lab is staffed by three senior researchers: Kees-Jan Weststrate (Fischer-Tropsch Chemistry), Hans Fredriksson (syngas & hydrogen) and Foteini Sapountzi (electrolysis), collaborating with SynCat@Beijing, DIFFER, and universities in Europe and South Africa.

A comprehensive review on electrocatalysts for syngas and hydrogen production is freely available in Progr. Energy Comb. Sci. 58 (2017) 1-35 (open access!)

Syngaschem BV offers short courses in personal development, summarized in our book Scientific Leadership; Jan-Karel Felderhof and Hans Niemantsverdriet, DeGruyter, Berlin (price € 29,95).

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