From Wind and Solar Energy to Chemical Energy Storage: Understanding and Engineering Catalysis under Dynamic Conditions

758. WE-Heraeus-Seminar

10 – 13 January 2022

ONLINE

WILHELM UND ELSE
HERAEUS-STIFTUNG

Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see https://www.we-heraeus-stiftung.de

Aims and scope of the 758. WE-Heraeus-Seminar:

The German Energy Transition ("Energiewende") aims at decreasing net emissions of CO_2 by 95 % and increase the renewable energy fraction to 60 % by 2050. Similar targets are aimed at in other European countries and around the globe. An important aspect in the future is storage in chemicals and the production of fuels and chemicals based on renewable sources, particular based on wind turbines and photovoltaic solar power. The idea is to transform low-energy molecules such as water and CO_2 into high-energy reactive molecules: hydrogen, hydrocarbons, oxygenates and fuels. In contrast to conventional resources, wind and solar power fluctuates on time scales of minutes to days – depending on season, time of day and weather. Processes in focus are water electrolysis into hydrogen and oxygen, as well as conversion of CO_2 into hydrocarbons and oxygenates including methane, methanol and CO. Primarily, these processes were developed and well-studied for steady-state applications. In order to understand and optimize them under fluctuating conditions, new catalyst concepts must be developed – a very challenging topic in catalysis.

Orchestrating the complex interplay between imposed dynamic operation conditions and a concomitant or intrinsic structural evolution of the working catalysts will require an unprecedented mechanistic understanding at the atomic scale. Besides traditional catalyst preparation and testing, novel hierarchical catalyst design, advanced characterization tools as well as detailed modeling and simulation approaches will become ever more important to this end. Research in this area thus embraces predictive - quality first - principles calculations, multiscale modeling, data science and analytics, operando spectroscopies and in situ microscopies, as well as kinetic measurements, materials and reactor design. This requires a strong interaction of scientists from physics, theory, chemistry and engineering.

Bringing scientists from these various disciplines together, this WE-Heraeus Seminar aims at presenting the current state of research and advances towards such dynamic operation of catalytic energy storage systems, with significant focus on the fundamental methods that drive this research.

Introduction

Scientific Organizers:

Prof. Dr. Jan-Dierk Grunwaldt — Karlsruhe Institute of Technology, Germany
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Prof. Dr. Roger Gläser — University of Leipzig, Germany
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Program

Program *(CET)*

Monday, 10 January 2022

Chair: Jan-Dierk Grunwaldt

08:30 – 08:40	Jan-Dierk Grunwaldt Roger Gläser Karsten Reuter	**Welcome**
08:40 – 09:35	Ulrike Diebold	**Fundamental Studies Using Surface Science Technique**
09:35 – 10:20	Petra de Jongh	**Design of Heterogeneous Catalysts**
10:20 – 10:45	*COFFEE BREAK / NETWORKING*	
10:45 – 11:30	Beatriz Roldan Cuenya	**From Clusters to Catalysts in Energy Storage**
11:30 – 12:15	Ib Chorkendorff	**Experimental Aspect of Electrochemical Ammonia Synthesis**
12 :15 – 12:30	Stefan Jorda	**About the Wilhelm and Else Heraeus Foundation**
12:30 – 14:00	*LUNCH BREAK / NETWORKING*	
14:00 – 14:45	Karl J. J. Mayrhofer	**Electrocatalysis**
14:45 – 15:30	Eranda Nikolla	**Electrocatalytic Reduction of CO_2**
15:30 – 16:00	*COFFEE BREAK / NETWORKING*	
16:00 – 16:45	Ulrike Krewer	**Modelling of Electrocatalytic Systems**
16:45 – 18:15	**Posterflash (1 min) and Poster Session I** (MeetAnyway)	

Program *(CET)*

Tuesday, 11 January 2022

Chair: Karsten Reuter

08:30 – 09:30	Robert Schlögl	**Future of Energy Storage in Chemicals**
09:30 – 10:15	Regina Palkovits	**CO_2-Hydrogenation and Oxymethylene Ethers**
10:15 – 10:45	*COFFEE BREAK / NETWORKING*	
10:40 – 11:30	Martin Muhler	**New Insights into Methanol Synthesis**
11:30 – 12:15	Nico Fischer	**Advanced Characterization and Understanding of Fischer-Tropsch Catalysts**
12:15 – 13:30	*LUNCH BREAK / NETWORKING*	
13:30 – 15:00	**Posterflash (1 min) and Poster Session II** (MeetAnyway)	
15:00 – 15:30	*COFFEE BREAK / NETWORKING*	
15:30 – 16:30	Ferdi Schüth	**Future Energy Scenarios**
16:30 – 18:15	Angelika Heinzel Andreas Förster Maximilian Fleischer Bert M. Weckhuysen	**Panel Discussion "Our Energy System in 2050"**

Program *(CET)*

Wednesday, 12 January 2022

Chair: Roger Gläser

08:30 – 09:30	Bert M. Weckhuysen	**Operando Spectroscopy and Microscopy in Catalysis**
09:30 – 10:15	Marc Willinger	**Advances in Electron Microscopy**
10:15 – 10:45	*COFFEE BREAK / NETWORKING*	
10:45 – 11:30	Mirijam Zobel	**In Situ/Operando Characterization Using Synchrotron Scattering Techniques**
11:30 – 12:30	Jens K. Nørskov	**Electrochemical Nitrogen Activation, Insights from Theory**
12:30 – 14:00	*LUNCH BREAK / NETWORKING*	
14:00 – 14:45	Jan Rossmeisl	**Predicting Electrocatalysis at the Atomic Scale**
14:45 – 15:30	Zachary W. Ulissi	**Continued Progress towards Generalizable Machine Learning Models in Computational Catalysis**
15:30 – 16:00	*COFFEE BREAK / NETWORKING*	
16:00 – 16:45	Olaf Deutschmann	**Novel Tools for Digitalization and Archiving of Experimental and Modelling Data in Reaction Kinetics**
16:45 – 17:45	Julia Schmoeckel (TBC)	**Weather Forecast and Renewable Energies**

Program *(CET)*

Thursday, 13 January 2022

Chairs: Karsten Reuter / Roger Gläser

08:30 – 09:15	Stephan Schunk	**Catalyst Design by Digitalization Approaches**
09:15 – 10:00	Anke Hagen	**Solid Oxide Electrolyzer under Dynamic Load for Hydrogen and Syngas Production**
10:00 – 10:30	*COFFEE BREAK / NETWORKING*	
10:30– 11:15	Roland Dittmeyer	**Decentralized Processes: Energy-Related Catalysis Using Modular Reactor Design**
11:15– 12:15	Gabriele Centi	**Outlook for CO_2-Reduction and Future Scenarios on a European Level**
12:15 – 12:30	Organizers	**Closing Remarks and Poster Prize**
12:30	*END OF THE SEMINAR*	

Posters

Poster Session II – Tuesday, 11 January 2022

12	Alexander Bodach *	**Hydrogen Activation by Al-N Lewis Pairs and Mechanochemical Syntheses of Organometallic Compounds**
13	Charlotte Fritsch *	**Development of a Ceramic Membrane Reactor for Coupled Propane Dehydration and Hydrogen Production**
14	Florian Hausen *	**Revealing Surface Transformations by operando Friction Force Microscopy**
15	Klara Sophia Kley *	**Selective Hydrogenation of High Concentrated Acetylene with Mechanochemical Prepared Pd-Ag/α-Al2O3 as a Catalyst**
16	Kevin Kuhlmann *	**Reactive CFD and NMR: Bringing Research Areas Together for Detailed, Full-Field Validation**
17	Xiaoran Liu *	**Al-N Compounds for Hydrogen Activation and as Energetic Materials**
18	Fei Wang *	**24/7 Dispatchable Solar Power System Powered by High Temperature Hydrogen Storage Materials**
19	Yonghyuk Lee	**Data-Efficient Iterative Training of Machine-Learning Gaussian Approximation Potentials for Surface Structure Determination of Living Heterogeneous Catalysts**
20	Felix Studt	**Theoretical Studies on the Conversion of Methanol to Olefins Using Acidic Zeolites**
21	Daliborka Nikolić	**Analysis of Possible Improvement of Forced Periodically Operated Chemical Reactor with Methanol Synthesis Based on Nonlinear Frequency Response Method**

Abstracts of Posters

(in alphabetical order)

Analysis of possible improvement of forced periodically operated chemical reactor with methanol synthesis based on Nonlinear Frequency Response Method

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Abstract

Forced periodic operations, as one way of Process Intensification, can be used in order to achieve better performances of chemical reactors, in comparison to conventional steady-state operation. In this study the Nonlinear Frequency Response (NFR) method, a powerful analytical and approximate tool which gives an answer whether and under which conditions certain periodic operation would lead to improvement of process performance was used. The analysis was done for the methanol synthesis using a standard Cu/ZnO catalyst performed in an isothermal and isobaric lab-scale CSTR. At first the single input modulations were analysed. The inputs considered for periodic modulation are: partial pressures of each reactant in the feed stream and the total volumetric inlet flow-rate. The objective was to maximize the mean molar outlet flow-rate of methanol. The specific forcing parameters were optimized. The results of the NFR analysis showed that modulations of single inputs do not provide potential for significant improvements.

The study was extended to analysis of periodic operations with simultaneous modulations of two inputs. Six possible input combinations were analysed and the optimal forcing parameters which maximizing again the time-average methanol production were determined. For all combinations an improvement is possible, but for some cases it was found to be not significant. However, significant improvements are predicted for a) simultaneous modulation of the partial pressure of CO_2 in the feed steam and the volumetric inlet flow-rate and b) simultaneous modulation of the partial pressure of hydrogen (H_2) and the volumetric inlet flow-rate [1, 2]. The highest improvement could be achieved for simultaneous modulation of the inlet partial pressure of CO and the inlet volumetric flow rate.

References:

[1] Nikolić, D., Seidel, C., Felischak, M., Miličić, T., Kienle, A., Seidel-Morgenstern, A., Petkovska, M., Chem. Eng. Sci., 2021, 117134

[2] Nikolić, D., Seidel, C., Felischak, M., Miličić, T., Kienle, A., Seidel-Morgenstern, A., Petkovska, M, Chem. Eng. Sci., 2021, 117133