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## Conference Program

### Saturday, September 07

**09:30-11:30 Registration**

**11:30-12:30 Lunch**

#### 12:30-12:50 Opening Remarks:

**Dr. Lisong Xiao** (Chair of GCCCD)

**Mr. Yunhua Lou** (First Secretary, Education Section, the Embassy of P.R. China in Germany)

**Ms. Hannelore Bossmann** (Head of Section China, Mongolia, DAAD)

**Dr. Zhong Hong** (General Manager of Coatings and Additives, Greater China Region, Evonik)

#### 12:50-14:40 Session 1: Nano Energy Chair: Dr. Xingxing Chen

**12:50-13:15** *Plasma synthesis of nanostructures for improved thermoelectric properties* (1.1)

Invited Speaker 1: Dr. Hartmut Wiggers

**13:15-13:40** *Carbon Nanomaterials in Electrochemical Energy Storage and Conversion* (1.2)

Invited Speaker 2: Dr. Wei Xia

**13:40-14:00** *Secondary Structured Silicon-Carbon Nanotube Hollow Spheres for High Capacity Lithium Ion Battery Anode Materials* (1.3)

Speaker 3: Dr. Pengfei Gao

**14:00-14:20** *CuO-CeO<sub>2</sub> catalysts for PROX reaction: Flame spray synthesis and EPR study* (1.4)

Speaker 4: Dr. Feng Wang

**14:20-14:40** *Size effects on lithium storage and phase transition in LiFePO<sub>4</sub>/FePO<sub>4</sub> system* (1.5)

Speaker 5: Dr. Changbao Zhu

#### 14:40-15:05 Coffee Break



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**15:05-16:30      Session 2: Organic/Bio-Chemistry      Chair: Dr. Jianwei Tong**

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**15:05-15:30**      *Rh<sup>III</sup>/Cu<sup>II</sup>-Cocatalyzed Synthesis of 1H-indazoles through C-H Amidation and N-N Bond Formation (2.1)*

Invited Speaker 3: Dr. Dagang Yu

**15:30-15:50**      *Ti-cis-DACH-salalen Catalyzed Asymmetric Epoxidation of Terminal, non-Conjugated Olefins with Aqueous H<sub>2</sub>O<sub>2</sub> (2.2)*

Speaker 7: Dr. Qifang Wang

**15:50-16:10**      *From CO<sub>2</sub> to Polyurethanes (2.3)*

Speaker 8: Dr. Mingyan Ma

**16:10-16:30**      *Selective Enrichment of Phosphopeptides with Molecularly Imprinted Polymers (2.4)*

Speaker 9: Jing Chen

**16:30-16:50      Coffee Break**

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**16:50-17:50      Session 3: Industry      Chair: Dr. Zhong Hong**

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**16:50-17:50**      *Opportunities & challenges for chemical companies in Asia*

Invited Speaker 4: Dr. Dahai Yu

**19:00-22:00      25<sup>th</sup> GCCCD Anniversary Banquet (Entrance starts 18:30)**

## Sunday, September 08

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**09:10-10:35      Session 4: Inorganic/Green Chemistry      Chair: Dr. Wei Xia**

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**09:10-09:35**      *Nanofabrication and Nanopatterning: Self Assembly of Metallic Particles, Organic Molecules, and Polyelectrolytes at Interface in Top-Down or Bottom-Up Fashion (4.1)*

Invited Speaker 5: Dr. Jianli Zhao



- 09:35-09:55**     *Hybrid photoanodes for visible light-driven water splitting* (4.2)  
Speaker 12: Dr. Lidong Wang
- 09:55-10:15**     *Tunable dual-mode photoluminescence from  $\text{Eu}^{2+}/\text{Eu}^{3+}$  activated silicate glass and glass ceramic phosphors* (4.3)  
Speaker 13: Guojun Gao
- 10:15-10:35**     *Carbon Nitrides materials in photocatalytic reactions* (4.4)  
Speaker 14: Dr. Hongji Wang
- 10:35-11:00**     **Coffee Break**
- 11:00-12:25**     **Session 5: Theoretical/Analytical Chemistry    Chair: Dr. Xiaoyan Cao-Dolg**
- 11:00-11:25**     *Molecular Photophysics and Photochemistry: Combining static electronic structure calculations and dynamics simulations* (5.1)  
Invited Speaker 6: Dr. Ganglong Cui
- 11:25-11:45**     *A powerful tool in rediscovery of Traditional Chinese Medicine: Multidimensional chromatography* (5.2)  
Speaker 16: Dr. Duxin Li
- 11:45-12:05**     *Bioleaching: a promising tool for metal winning* (5.3)  
Speaker 17: Ruiyong Zhang
- 12:05-12:25**     *Global innovation for value creation in a multinational company* (5.4)  
Speaker 18: Dr. Zhong Hong
- 12:25-12:40**     **Closing remark** **Dr. Lisong Xiao**
- 13:00**            **Leaving**

## Abstracts

### Section 1: Nano Energy

#### **1.1 Plasma synthesis of nanostructures for improved thermoelectric properties**

Hartmut Wiggers

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The continuous and increasing discussion regarding possibilities for energy harvesting, power efficiency and sustainability has led to an intensive (re)search for further development and optimization of energy conversion processes. This covers all areas from improvement in efficiency over improved insulation techniques to waste heat recovery. The latter one becomes more and more interesting as new approaches in thermoelectrics pave the way for its commercialization. Thermoelectric materials are solids, which allow for a direct conversion of temperature differences into electrical energy. Thermoelectric generators have proven to show long-term stability and reliability even under extreme conditions but up to now they are mainly used in niche applications like space probes or at remote locations. Despite of still relatively low over-all performance with respect to costs and efficiency, thermoelectrics are highly interesting for heat recovery, especially at high-temperatures such as waste heat from processing plants or from automobile exhaust, containing about 30% of the overall energy delivered from the fuel.

The utilization of nanoscale silicon-based materials for high temperature thermoelectrics is studied with respect to synthesis and processing of doped silicon nanoparticles from gas phase plasma synthesis. It is found that plasma synthesis enables for the formation of spherical, highly crystalline and soft-agglomerated materials. The requirements for the formation of dense sintered bodies while keeping the crystallite size small will be discussed. Both, small particles sizing a few ten nanometer and below that are easily achievable from plasma synthesis, and a weak surface oxidation lead to a pronounced sinter activity about 350 K below the temperature usually needed for successful densification of silicon. The thermoelectric properties of our sintered materials are comparable with the best results found for nanocrystalline silicon prepared by other methods than plasma synthesis.

#### References:

1. Kessler, V., Gautam, D., Hülser, T., Spree, M., Theissmann, R., Winterer, M., Wiggers, H., Schmechel, R., *Advanced Engineering Materials*, 15 (2013) 379-385.
2. N. Stein, N. Petermann, R. Theissmann, G. Schierning, R. Schmechel, H. Wiggers, *J. Mater. Res.*, 26 (2011) 1872–1878.
3. N. Petermann, N. Stein, G. Schierning, R. Theissmann, B. Stoib, M. S. Brandt, C. Hecht, C. Schulz, H. Wiggers, *J. Phys. D: Appl. Phys.*, 44 (2011) 174034.
4. G. Schierning, R. Theissmann, N. Stein, N. Petermann, A. Becker, M. Engenhorst, V. Kessler, M. Geller, A. Beckel, H. Wiggers, R. Schmechel, *J. Appl. Phys.*, 110 (2011) 113515.



## 1.2 Carbon Nanomaterials in Electrochemical Energy Storage and Conversion

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Sustainable development requires the development of renewable energy sources and the increase of energy efficiency. Decentralized energy supply from solar irradiation, wind, or hydropower strongly relies on the conversion and storage of energy in different forms, for example, (1) storage of electrical energy in form of hydrogen through electrolysis; (2) storage of electrical energy in batteries; (3) using solar energy to produce hydrogen through photocatalytic water splitting; (4) the recovery of electrical energy from hydrogen or hydrocarbons using fuel cells. These processes can be translated to the following chemistry: (a) oxygen reduction reaction in fuel cells, metal-air batteries; (b) oxygen evolution reaction in H<sub>2</sub>O electrolysis, metal-air batteries; (c) lithium storage in carbon in batteries.

Carbon nanomaterials are widely used in electrochemistry due to their unique structure, high conductivity and chemical resistance. For example, carbon black is used as conductive additive and catalyst support, and graphite is used as anode material for lithium storage. Carbon nanotubes (CNTs) have both a highly crystalline structure and a high surface area. The electrochemical and thermal stability of CNTs is significantly higher than that of other high-surface carbon materials like carbon black or active carbon. Carbon materials have the major advantage that their surface properties can be tuned with great precision. Surface defects, functional groups and heteroatoms can be created on or incorporated in carbon surfaces in a controlled manner. Doping of carbon represents one of the major interests in current research. Nitrogen-doped carbon materials were used as metal-free catalysts and showed extraordinary catalytic activities in the oxygen reduction reaction especially under alkaline conditions.

### References:

1. E. Ventosa, P. Chen, W. Schuhmann, W. Xia, *Electrochem. Commun.* 25 (2012) 132.
2. A. Zhao, J. Masa, M. Muhler, W. Schuhmann, W. Xia, *Electrochim. Acta* 98 (2013) 139.
3. M. S á nchez, P. Chen, T. Reinecke, M. Muhler, W. Xia, *ChemCatChem* 4 (2012) 1997.
4. J. Masa, A. Bordoloi, M. Muhler, W. Schuhmann, W. Xia, *ChemSusChem* 5 (2012) 523.

### 1.3 Secondary Structured Silicon-Carbon Nanotube Hollow Spheres for High Capacity Lithium Ion Battery Anode Materials

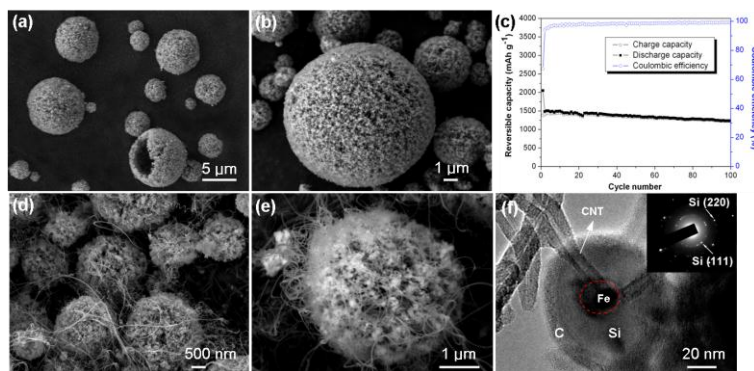
Pengfei Gao<sup>a</sup>, Jun Yang<sup>b</sup>

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Recently, silicon-based materials have received particular interest for their high specific capacity for lithium storage than that of conventional graphite<sup>1</sup>. Great efforts have been made to design nano/micro-structured silicon-based composites so as to accommodate the large volume effect of silicon and to achieve stable performance. Generally speaking, the synthetic routes to get hierarchical nano/micro-architectures are sophisticated and not suitable for large-scale production. Herein, we report the fabrication of a hollow sphere secondary structured silicon-carbon nanotube composite via a facile template-free method.



**Fig. 1** (a, b) SEM images of the silicon-iron nitrate hollow spheres. (c) Cycling performance of the Si-CNT@C hollow sphere electrode. (d, e) SEM images of the Si-CNT@C hollow spheres. (f) TEM image of the Si-CNT-C junction and the SAED pattern.

For a typical synthesis, the commercial 100 nm-sized silicon nanoparticles were dispersed in the iron nitrate solution in water-ethanol mixed solvents. The silicon-iron nitrate hollow spheres (Fig. 1a, b) were obtained by spray pyrolysis of the mixture at 170 °C. Then CNTs were grown from the inside of the hollow spheres via a Chemical Vapor Deposition (CVD) process at 750 °C using C<sub>2</sub>H<sub>2</sub> as the carbon source. Furthermore, we coated the material with carbon to strengthen the whole structure. Fig. 1d, e, f showed the morphology and microstructure of the as-prepared silicon-carbon nanotube hollow spheres (Si-CNT@C). The Si-CNT@C displayed an initial reversible capacity of 1380 mAh g<sup>-1</sup> and remained over 1200 mAh g<sup>-1</sup> even up to 100 cycles (Fig. 1c).

This superior cycling performance can be ascribed to the hollow space as well as the flexible CNTs which accommodated the silicon expansion and contraction during cycling. This convenient method should be also suitable for preparing other materials with hollow sphere structures for electrochemical energy conversion and storage applications.

#### References:

1. Wu, H.; Cui, Y. *Nano Today* 2012, 7, 414.

## 1.4 CuO-CeO<sub>2</sub> catalysts for PROX reaction: Flame spray synthesis and EPR study

Feng Wang, B üchel Robert, Anton Savitsky, Sotiris E. Pratsinis, Wolfgang Lubitz and Ferdi Sch üth

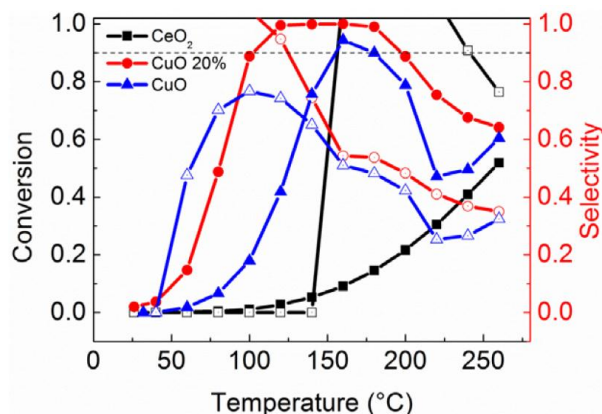
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Preferential oxidation of CO (PROX) is used to remove CO from a H<sub>2</sub> containing gas stream. The CO needs to be removed, otherwise it will poison the catalysts of the polymer-electrolyte membrane fuel cell (PEMFC). For PROX, CuO-CeO<sub>2</sub> is currently the most promising catalysts system showing high conversion and selectivity between 100 - 200 °C. In general, such catalysts have been prepared by suspension/co-precipitation, in H<sub>2</sub> atmosphere impregnation, microemulsion, and nanocasting.

Catalysts with >99% conversion and >70% selectivity have been reported, but their operation window is still very narrow, at best 18 °C, requiring a precise temperature control during the PROX reaction. In-situ DRIFTS and XANES study showed that CO oxidation takes place at interfacial positions of the dispersed Cu<sup>2+</sup> species and H<sub>2</sub> oxidation occurs at surface Cu<sup>+</sup> sites. EPR study showed that surface Cu<sup>2+</sup> dimers are active sites for CO adsorption and maybe oxidation. The criteria for a good CuO-CeO<sub>2</sub> system are: 1) high concentration of Cu<sup>2+</sup> dimers on the surface, 2) high surface area, 3) preferably a wide operation window for PROX.

In this report, we show that: 1, Flame pyrolysis method can prepare 5-nm CuO-CeO<sub>2</sub> nanocrystals with up to 200 m<sup>2</sup>/g BET surface area. 2, The operation window was extended to 27 °C, which will be suitable for industrial application. 3, Surface Cu<sup>2+</sup> dimers were identified through EPR studies. 4, In-situ EPR measurement determined the Cu<sup>2+</sup> dimers' behaviors during the catalysis process. We also have noticed that in-situ EPR measurement for CO oxidation reactions have never been carried out before. By looking into details of the CuO-CeO<sub>2</sub> systems, more efficient catalysts could be designed for industrial PROX reactions.



**Figure 1.** Conversion and selectivity of CeO<sub>2</sub>, CuO and 20wt% CuO-CeO<sub>2</sub> catalysts in PROX reactions.

### References:

1. H. Yen, Y. B. Seo, S. Kaliaguine, F. Kleitz, *Angew. Chem. Int. Ed.* 51 (2012) 12032.
2. A. Tsch öpe, W. Liu, M. Flytzani-Stephanopoulos, J. Y. Ying, *J. Cata.* 157 (1995) 42.





## 1.5 Size effects on lithium storage and phase transition in LiFePO<sub>4</sub>/FePO<sub>4</sub> system

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Recently, LiFePO<sub>4</sub> has received much attention as a potential of high rate cathode material for electric vehicle and hybrid electric vehicle. However, size effects in LiFePO<sub>4</sub> need to be clarified in order to arrive at deeper conceptual understanding of its electrochemical behaviour.

In this work, the carbon-coated single-crystalline LiFePO<sub>4</sub> nanowires<sup>1</sup> and size-controlled LiFePO<sub>4</sub> nanoparticles were successfully prepared. The lithium potential variations are systematically investigated in metastable LiFePO<sub>4</sub> (e.g. nanocrystalline LiFePO<sub>4</sub> with different particle sizes and amorphous LiFePO<sub>4</sub>) thermodynamically and experimentally. Apparent shrinkage of the miscibility gap and decrease of OCV values by reducing the particle size were confirmed. The effect of size as well as the impact of amorphization are strongly dependent on the storage mechanism (single phase vs. two phase model), size distribution and surface energy.

The thermodynamic effects in the LiFePO<sub>4</sub> are very complex and even staging phenomena<sup>2</sup> are observed during phase transition process, which challenges the traditional two phase models. Various staging phenomena were observed for LiFePO<sub>4</sub> of different sizes. The corresponding thermodynamics and kinetics for phase transition process are discussed.

### Reference:

1. C. Zhu, Y. Yu, L. Gu, K. Weichert, and J. Maier, *Angew. Chem. Int. Ed.*, 50, 6278 (2011).
2. L. Gu, C. Zhu, H. Li, Y. Yu, C. L. Li, S. Tsukimoto, J. Maier, and Y. Ikuhara, *J. Am. Chem. Soc.*, 133, 466 (2011).

## Section 2: Organic/Bio-Chemistry

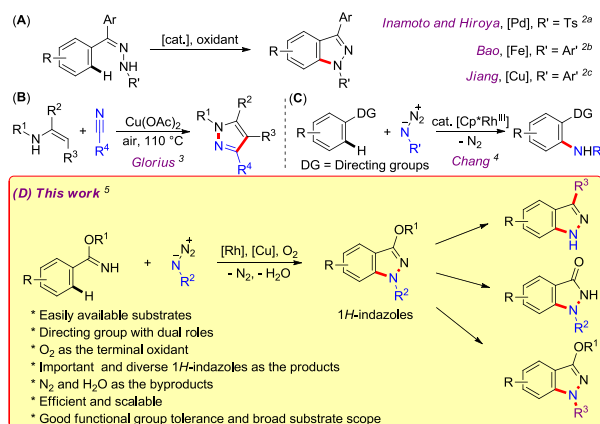
### 2.1 Rh<sup>III</sup>/Cu<sup>II</sup>-Cocatalyzed Synthesis of 1*H*-indazoles through C-H Amidation and N-N Bond Formation

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Due to the diverse pharmacological activities, 1*H*-indazoles are widely used as anticancer, -inflammatory, and -microbial drugs.<sup>1</sup> Therefore, the efficient synthesis of 1*H*-indazoles has attracted much attention for a long time.<sup>2</sup> Recently, transition-metal-catalyzed C-H activation has become more and more powerful and has been playing an important role in the synthesis of heterocycles, including 1*H*-indazoles. Starting from arylhydrazones, palladium<sup>2b</sup>, iron<sup>2c</sup> and copper<sup>2d</sup> catalysts were used to synthesize 1*H*-indazoles through C-H amination. However, toxic organohydrazines have to be used and the substrates are limited to diarylketone derivatives. Based on previous works of Chang's<sup>3</sup> and our group<sup>4</sup>, a novel synthesis of substituted 1*H*-indazoles from easily available arylimidates and organoazides via Rh-catalyzed C-H activation/C-N bond formation and Cu-catalyzed N-N bond formation is reported herein.<sup>5</sup> The corresponding 1*H*-indazoles were obtained in moderate to excellent yields with good functional group tolerance. The process is green with N<sub>2</sub> and H<sub>2</sub>O as the byproducts. Moreover, the products could also be further transferred to other important derivatives.



#### Reference:

- (1) E. Barile, S. K. De, C. B. Carlson, V. Chen, C. Knutzen, M. Riel-Mehan, L. Yang, R. Dahl, G. Chiang, M. Pellecchia, *J. Med. Chem.* 2010, 53, 8368 and reference therein.
- (2) a) K. Inamoto, T. Saito, M. Katsuno, T. Sakamoto, K. Hiroya, *Org. Lett.* 2007, 9, 2931. b) T. Zhang, W. Bao, *J. Org. Chem.* 2013, 78, 1317. c) X. Li, L. He, H. Chen, W. Wu, H. Jiang, *J. Org. Chem.* 2013, 78, 3636.
- (3) a) J. J. Neumann, M. Suri, F. Glorius, *Angew. Chem. Int. Ed.* 2010, 49, 7790. b) M. Suri, T. Jousseume, J. J. Neumann, F. Glorius, *Green Chem.* 2012, 14, 2193.
- (4) a) J. Y. Kim, S. H. Park, J. Ryu, S. H. Cho, S. H. Kim, S. Chang, *J. Am. Chem. Soc.* 2012, 134, 9110. b) J. Ryu, K. Shin, S. H. Park, J. Y. Kim, S. Chang, *Angew. Chem. Int. Ed.* 2012, 51, 9904.
- (5) This work: D.-G. Yu<sup>†</sup>, M. Suri<sup>†</sup>, F. Glorius, *J. Am. Chem. Soc.* 2013, 135, 8802. (<sup>†</sup> equal contribution)

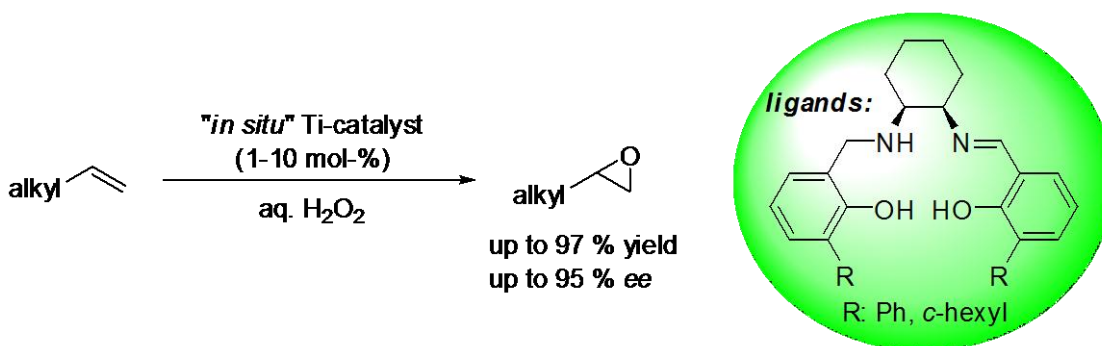
## 2.2 Ti-*cis*-DACH-salalen catalyzed asymmetric epoxidation of terminal, non-conjugated olefins with aqueous H<sub>2</sub>O<sub>2</sub>

Qifang Wang and Albrecht Berkessel\*

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Optically active epoxides are high-utility molecules in synthetic organic chemistry. Thus many efforts have been devoted to the development of efficient catalyst systems for the preparation of enantiomerically enriched epoxides. Asymmetric epoxidation of olefins is the most direct approach.<sup>1</sup> In 2005, *Katsuki et al.* introduced Ti-salalen complexes as the novel and highly enantioselective catalysts for the asymmetric epoxidation of a variety of non-functionalized olefins using aqueous H<sub>2</sub>O<sub>2</sub> as the oxidant.<sup>2</sup>



Our own work in this area aimed at simplifying the catalyst complexes,<sup>3</sup> while retaining its remarkable ability for the asymmetric epoxidation of non-conjugated olefins. We have developed a versatile synthetic route for the salalen ligands with *cis*-DACH as the chiral backbone. *Cis*-DACH-salalen ligands derived Ti-complexes are particularly well suited for terminal non-conjugated olefins and provide high yields and enantioselectivities (up to 95% ee), using our improved *in situ/vac* procedure with aqueous H<sub>2</sub>O<sub>2</sub> as the oxidant.<sup>4</sup>

### References:

1. Reviews on asymmetric epoxidation: a) K. Matsumoto, T. Katsuki in "Catalytic Asymmetric Synthesis", 3rd ed. (I. Ojima, Ed.), Wiley, Hoboken, USA, 2010, pp. 839-890; b) Q.-H. Xia, H.-Q. Ge, C.-P. Ye, Z.-M. Liu, K.-X. Su, *Chem. Rev.* 2005, 105, 1603-1662.
2. a) K. Matsumoto, Y. Sawada, B. Saito, K. Sakai, T. Katsuki, *Angew. Chem. Int. Ed.* 2005, 44, 4935-4939; b) Y. Sawada, K. Matsumoto, T. Katsuki, *Angew. Chem. Int. Ed.* 2007, 46, 4559-4561.
3. a) A. Berkessel, M. Brandenburg, E. Leitterstorf, J. Frey, J. Lex, M. Schfer, *Adv. Synth. Catal.* 2007, 349, 2385-2391; b) A. Berkessel, M. Brandenburg, M. Schfer, *Adv. Synth. Catal.* 2008, 350, 1287-1294.
4. A. Berkessel, T. Gnther, Q. Wang, J.-M. Neudrfl, *Angew. Chem. Int. Ed.* 2013, 52, 8467-8471.

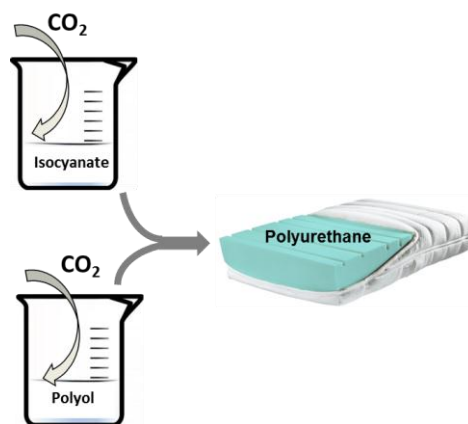
## 2.3 From CO<sub>2</sub> to Polyurethanes

Mingyan Ma, Walter Leitner, Christoph Gürtler and Thomas E. Müller

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Carbon dioxide (CO<sub>2</sub>) is an abundant and economic resource. Using the climate gas CO<sub>2</sub> to generate advanced polyurethane materials, which are among the most well-known polymers and widely used in foam, coating, paint and adhesive industries, is undoubtedly a sustainable way for CO<sub>2</sub> utilization and polyurethane industry.<sup>1</sup>



Isocyanates and polyols are the two main raw materials for producing polyurethanes. In our present research, CO<sub>2</sub>-based routes are developed for synthesizing both isocyanates and polyols, which enable us to produce more environmentally beneficial polyurethane materials.

### References

1. T. E. Müller, W. Leitner, et al. *ChemSusChem*, 2011, 4, 1216.



## 2.4 Selective Enrichment of Phosphopeptides with Molecularly Imprinted Polymers

<sup>1</sup>Jing Chen, <sup>1</sup>Stefan Helling, <sup>2</sup>Sudhirkumar Shinde, <sup>2</sup>Börje Sellergren, <sup>1</sup>Katrin Marcus

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Phosphorylated proteins are very important in intracellular signal transduction processes and their analysis forms an important part of proteomics research, drug discovery and disease diagnostics. Phosphoproteins are mostly characterized by using mass-spectrometry (MS) methods after proteolytic processing, however phosphopeptides are notoriously difficult to analyze by MS, especially in presence of non-modified peptides.

Aim of the work is to apply the phosphor-tyrosine and phosphor-serine single amino acid imprinted polymers (pY-MIP, pS-MIP) as well as a peptide sequence imprinted polymer to selectively enrich phosphopeptides using solid phase extraction (SPE) method.

Peptide mixture standard was used as a sample mixture with. Pipette tips with C8 membrane plug at the bottom were filled with ca. 1mg MIP as the stationary phase for a self-made micro column<sup>1</sup>. SPE steps were carried out and fractions of flow through, washing, elution measured on MALDI-TOF/TOF-MS (Bruker, Ultraflex II), quantified by Flexanalysis (Bruker).

New generation of the peptide sequence specific MIP was synthesized and used as a plastic antibody to enrich the HtrA<sub>2</sub>/Omi peptide related to Parkinson Disease<sup>2</sup>. After the crude determination from the SPE procedure with standard peptide mixture, conditions will be applied to biological sample -- trypsin digested mouse brain samples within which the HtrA<sub>2</sub>/Omi protein is over-expressed. The eluting fraction will be measured by HPLC-MS (Orbitrap Q-Exactive ) for further quantification of the targeted protein.

Results from the single amino acid imprinted polymer pTyr-MIP show clear discrimination of phosphotyrosine from phosphoserine peptides. Study of the peptide sequence imprinted polymer shows clear rebinding ability for the targeted peptide.

### References:

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2. Héliane Plun-Favreau et al., *Nature Cell Biology*, 2007, Vol. 9, No. 11, 1243-1252.



## **Section 3: Industry**

### ***Opportunities & challenges for chemical companies in Asia***

Dahai Yu

Member of the Executive Board of Evonik Industries AG and co-founder of the GCCCD

Evonik Industries AG, Essen, Germany

Asia is one of the world's most important growth regions. It has enormous economic potential, although the long-term growth projections for individual countries vary widely, which means that each nation has its own challenges to overcome. Growth rates in China have been dropping, but in global comparison are still significantly above the average GDP growth of 3% with a GDP growth of 7-8%. Key sectors for the chemical industry such as the automotive and construction industry continue to show high growth rates compared to developed countries. The specialty chemicals market is also growing much faster in Asia than in mature markets. In 2010, China's share of the global specialty chemicals market was 18%. This share is projected to increase to 24% by 2018, making the country the world's second largest market after Europe. Accordingly, China is an important growth driver for the global economy.

Furthermore, countries such as China and India have recognized the relevance of research and development for maintaining competitiveness in global competition. China's R&D budget now by far exceeds that of the high-tech country Japan. At the same time, educational levels are on the rise, giving China a large pool of highly qualified workers. Multinational companies that are continuously expanding their local presence therefore have targeted access to skilled Chinese workers and executives. Such international companies also offer excellent job opportunities for highly-qualified and well-trained executives.

For a globally leading specialty chemicals company like Evonik, which has aligned its strategy with the megatrends of health, nutrition, resource efficiency, and globalization, Asia—and particularly China—is an interesting key market. Additionally, China is a second home market for Evonik. The megatrends listed above have an enormous impact on the end-user markets of Evonik. Taking the example of resource efficiency, Asia will be the largest market for wind energy by the year 2020, and demand for locally manufactured, technologically advanced products is growing.

Evonik has over eighty years of experience in Asia and has consistently expanded its presence in the region. We now employ over 4,500 people at 23 sites in Asia and posted revenues of €2.4 billion in 2012. Local research and development is a high priority for Evonik to help understand the requirements of customers and to adapt products to special market requirements. The Group is therefore consistently expanding its presence on site by broadening its local production. By 2020, the Asian share of the company's revenue will be 30%. For that purpose, we are increasing the share of local production to 60% by 2015 and plan to invest €2 billion by then. Plans call for hiring another 2,000 employees by 2015 to adequately accompany this expansion of activities. Evonik is currently building three facilities in China, including a production complex for isophorones and isophorone diamine and an integrated production facility for organic specialty surfactants in Shanghai, a production plant for hydrogen peroxide in Jilin province, and a methionine production facility in Singapore.

## Section 4: Inorganic/Green-Chemistry

### 4.1 Nanofabrication and Nanopatterning: Self Assembly of Metallic Particles, Organic Molecules, and Polyelectrolytes at Interface in Top-Down or Bottom-Up Fashion

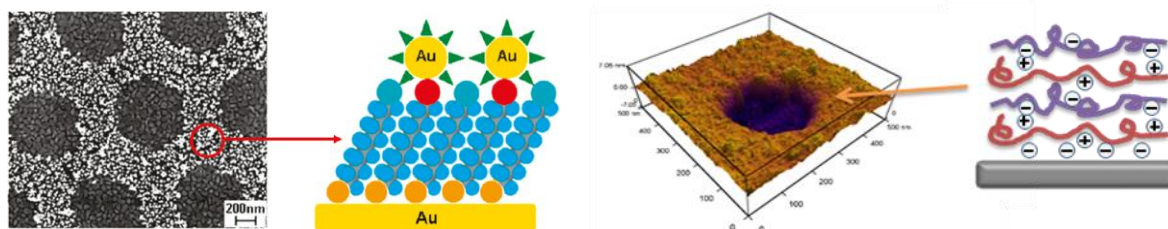
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Nanofabrication, defined as the design and manufacture of devices with nanometer-scale dimensions, has been one of the core aspects of nanoscience and elucidated new frontiers in science, medicine, and engineering for decades. Nanopatterning has now become firmly established in its own right as one of the principle and focused subdisciplines within nanofabrication. This still young field of nanotechnology has already undergone major advances and breakthroughs, which brings immense changes in the physical and chemical properties of a material by miniaturization of traditional micrometer-scale structures. Nanopatterning has been successfully engineered in top-down and bottom-up approaches. The former one was developed based on the traditional patterning techniques, while the latter one emerged recently taking advantage of the localized assembly of atoms, molecules or nanoobjects. For this purpose, a variety of lithographies have been used to (pre)pattern the surfaces for the following formation of nanostructures thereon.

In combination with my research, electron beam, UV, colloidal lithographies will be introduced for the fabrication of micro-, submicro-, and nanostructures utilizing metallic nanoparticles, organic molecules, and polyelectrolytes as building blocks. The diversity and difference among these techniques will also be briefly reviewed.



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## 4.2 Hybrid photoanodes for visible light-driven water splitting

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The development of photochemical systems capable of splitting water into hydrogen and oxygen has attracted significant interest motivated by the need to secure the future supply of clean and sustainable energy<sup>1</sup>. Due to the complex chemistry involved in four-electron oxidation of water to dioxygen<sup>2</sup>, the major challenge in photoelectrochemical water splitting is the development of cheap, efficient and stable photoanodes. Recently, we have been developing photoanodes based on a novel class of visible-light photoactive inorganic/organic hybrid materials –TiO<sub>2</sub> modified at the surface with polyheptazine (also known as “graphitic carbon nitride”). As we have shown, the optical absorption edge of the TiO<sub>2</sub>-polyheptazine hybrid is red-shifted into the visible (2.3 eV; ~540 nm) as compared to the bandgaps of both of the single components – TiO<sub>2</sub> (3.2 eV; ~390 nm) and polyheptazine (bandgap of 2.9 eV; ~428 nm), which is due to the formation of an interfacial charge-transfer complex between polyheptazine (donor) and TiO<sub>2</sub> (acceptor)<sup>3</sup>. In other words, the direct optical charge transfer leads to generation of electrons with a relatively negative potential in the conduction band of TiO<sub>2</sub>, while the holes photogenerated in the polyheptazine layer can drive photooxidation of water, as evidenced by visible light-driven evolution of dioxygen on hybrid electrodes modified with iridium or cobalt oxide nanoparticles acting as oxygen evolution co-catalysts<sup>3-5</sup>. Importantly, polyheptazine is highly stable, and at the same time it offers a possibility for further functionalization with transition metal-based catalytic sites enabling chemical transformations along multi-electron pathways. Our current attempts at improving the efficiency of kinetic charge separation in such hybrid photoanodes will be discussed.

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### 4.3 Tunable dual-mode photoluminescence from $\text{Eu}^{2+}/\text{Eu}^{3+}$ activated silicate glass and glass ceramic phosphors

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Inorganic materials doped with Rare earth (RE) ions have attracted extensive attention over recent decades owing to their wide applicability in phosphors, imaging, lasers and displays. Silicate glasses and especially the corresponding glass ceramics are used as host materials for RE ions due to their easy fabrication, broad compositional flexibility, high homogeneity, well-controlled dopant concentration, and good optical activity for dopants.<sup>1-3</sup>

Tunable dual-mode and enhanced PL of mixed valence  $\text{Eu}^{3+}/\text{Eu}^{2+}$  doped silicate glasses and glass ceramics are investigated. A glass ceramic route of reducing  $\text{Eu}^{3+}$  to  $\text{Eu}^{2+}$  is demonstrated. During the controlled nucleation and crystallization processes in a normal atmosphere,  $\text{Eu}^{3+}$  ions are partially incorporated into the newly deposited crystalline phases, (i.e.,  $\text{BaAl}_2\text{Si}_2\text{O}_8/\text{LaBO}_3$  and  $\text{Li}_2\text{ZnSiO}_4$ ), and gradually reduced to  $\text{Eu}^{2+}$  due to the charge compensation effect. Furthermore, it is investigated how to obtain and control the band-type blue PL of  $\text{Eu}^{2+}$  and the line-type red PL of  $\text{Eu}^{3+}$  in these glass ceramics by tunable ratio of  $\text{Eu}^{2+}/\text{Eu}^{3+}$ . A mechanism for the internal reduction of  $\text{Eu}^{3+}$  to  $\text{Eu}^{2+}$  is proposed. For  $\text{SiO}_2\text{-Al}_2\text{O}_3\text{-B}_2\text{O}_3\text{-BaO-La}_2\text{O}_3$  (SABBL) glass and corresponding  $\text{BaAl}_2\text{Si}_2\text{O}_8/\text{LaBO}_3$  glass ceramics, crystallization at elevated temperatures also results in the enhancement of PL intensity and PL lifetime of  $\text{Eu}^{3+}:^5\text{D}_0$  state.  $\text{Eu}^{3+}$  species are mostly incorporated on  $\text{La}^{3+}$  sites in  $\text{LaBO}_3$  crystallites, whereas the  $\text{Eu}^{2+}$  ions are located on  $\text{Ba}^{2+}$  sites in the hexacelsian phase. For  $\text{SiO}_2\text{-Li}_2\text{O-ZnO-Al}_2\text{O}_3\text{-K}_2\text{O-P}_2\text{O}_5$  (SLZAKP)  $\text{Li}_2\text{ZnSiO}_4$  glass ceramic, tunable dual-mode PL can be generated. The resulting PL color, ranging from orange/red to blue, can be tuned by adjusting the annealing temperature and the degree of crystallization.

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## 4.4 Carbon Nitrides materials in photocatalytic reactions

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Semiconductor photocatalyst development promises a clean, cheap and ethically-sound relief to global energy demands and climate change. Since Fujishima and Honda first reported the decomposition of water on illuminated TiO<sub>2</sub> electrodes in 1972,<sup>1</sup> technologies such as photocatalytic water splitting to produce hydrogen are seeing increasing importance for researchers. Apart from TiO<sub>2</sub>, metal-free (g-C<sub>3</sub>N<sub>4</sub>) carbon nitrides<sup>2</sup> are also promising semiconductor photocatalysts. These polymeric semiconductors are easily synthesized, have high thermal stability, are highly functional and show significant visible-light photocatalytic activity. The main focuses of this presentation are what is carbon nitrides, the synthesis and characterization of carbon nitrides and the photocatalytic properties of carbon nitrides.

In literature, melon was prepared in vacuum or nitrogen at temperatures between 560 and 600 °C for 12 – 36 h, or in an open system at 490 °C for 72 h.<sup>3,4</sup> Recently, it has been reported by Liu et al.<sup>5</sup> that melon prepared in an open system furnished graphene-like nanosheets by direct thermal oxidation. The resultant nanosheets possess a large surface area and show superior photocatalytic activities compared to bulk melon. Hereby, we have chosen to extend the calcination time at different temperatures in order to get large surface area ultra-long calcined melamine which could possess graphene-like carbon nitride nanosheets. And for this graphene-like materials also show good photocatalytic activities for the hydrogen evolution reaction driven by visible light.

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## **Section 5: Theoretical/Analytical-Chemistry**

### **5.1 Molecular Photophysics and Photochemistry:**

#### **Combining static electronic structure calculations and dynamics simulations**

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Photophysical and photochemical processes are ubiquitous in many areas, such as photodynamic therapy, natural and artificial water-splitting systems, dye-sensitized solar cell, photo-induced organic and inorganic reactions, chemical and bio-luminescence, light-emitting diodes, etc. Theoretical studies on these processes in particular at the atomic level is very important for us to understand the underlying working mechanisms, to control or tailor certain processes, and even to design better systems reversely.

In our theoretical studies, a strategy of combining static electronic structure calculations and dynamics simulations is used. The former can always provide valuable mechanistic insights, e.g. absorption and emission spectra, transition states, conical intersections, crossing points, decay channels, etc. However, dynamical information is totally lost, such as excited-state lifetimes, product distributions, competition and interplay among possible deactivation channels, etc., which call for a full-dimensional dynamics simulation.

In this talk I will present three our recent works in biological, organic, and inorganic areas: ortho-substituted green fluorescent protein (o-GFP) chromophore<sup>1</sup>, photo-induced Wolff rearrangement (WR) reaction<sup>2</sup>, and light-induced Au-Au bonding in oligomers<sup>3</sup>. (1) It is commonly known that for natural GFP chromophores in solution, excited-state decay is mainly related to the central double-bond isomerization, without proton transfer and with ca. 50% quantum yield for cis-trans isomerization. In this newly synthesized o-GFP, an ultrafast excited-state proton transfer and small cis-trans quantum yield (5%) have been observed in experiments. Our theoretical study explains well these intriguing photochemical phenomena. (2) Photoinduced WR reaction was discovered a century ago; but, its mechanism is still under debate until now. By means of a massive 1-picosecond nonadiabatic dynamics simulations and 10-picosecond BOMD dynamics simulations, the detailed mechanisms have been gained. (3) the Au(I) compounds in aqueous solution are bound to each other via a weak non-covalent aurophilic interaction; upon irradiation, however, a much stronger Au-Au chemical bond is formed. The physical origin for this interesting light-induced metal-metal chemical bonding has been revealed very recently by us.

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## 5.2 A powerful tool in rediscovery of Traditional Chinese Medicine: Multidimensional chromatography

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Anybody, during his whole life, may get sick and it is necessary to see a doctor whether Western or Traditional Chinese Medicine (TCM) practitioners. There are a big difference between two therapeutic theories and use of medicines, just as the cultural conflict between the west and east. For the medicine, normally pure compound with explicit validation was adopted in western medicine, while herbal medicine with hundreds of compound and more often herbal formula with thousands of largely unknown chemical composition were employed in TCM<sup>1</sup>. Bridging the gap between western medicine and TCM, multiple research strategies were proposed, like system biology<sup>2</sup>, herbalome<sup>3</sup>. Among these strategies, to make certain the bioactive compound/s by chromatographic methods is the key step. Traditional high performance liquid chromatography (HPLC) or more up-to-date ultra-high performance LC (UHPLC) presents insufficient efficiency in characterization of complex sample. A more powerful technique is needed to separate TCM samples, also in demand in proteomics, metabolomics and polymers.

Two-dimensional liquid chromatography (2DLC) has shown its powerful ability in the separation of complex sample since the first implementation in 1978 and is optimized by many other authors in the last decade in consideration of configuration, theoretical and application aspects<sup>4</sup>. A 2DLC comprises of two separation columns which are coupled online via an interface. The interface is usually a ten or eight-port switching valve with two equivalent sampling loops or trapping columns, operating in alternating cycles. The eluents from first dimensional elution were collected in the loop or trapping columns and subsequently transferred into the second dimensional separation column. Sample undergoes two separation mechanisms and thereby gets increased peak capacity, selectivity and resolution. Therefore, characterization of herbal medicine with this technique produces more information on chemical and structural composition.

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### 5.3 Bioleaching: a promising tool for metal winning-Biofilm formation and EPS analysis of leaching archaea

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Microbial leaching of metal sulfides (MS), recovery of valuable metals by using of acidophilic microorganisms, is a successful and expanding biotechnology<sup>1</sup>. However, it can occur as unwanted natural process namely acid rock drainage (ARD) or acid mine drainage (AMD). This process is accompanied with acidification and heavy metal pollution of water bodies and can cause serious environmental problems. Acidophilic archaea including genera such as *Ferroplasma*, *Acidianus*, *Sulfolobus* and *Metallosphaera* play important roles in bioleaching and AMD systems, and are being gained significant attention in commercial applications<sup>2-4</sup>.

Biofilms are defined as surface associated colonies of microorganisms embedded in extracellular polymeric substances (EPS)<sup>5</sup>. The attachment, colonisation and biofilm formation of microorganisms on MS is an important step in the bioleaching process. To date, limited information is available on the EPS composition and biofilms of archaeal species, especially concerning the ones grown on acidic environments<sup>6</sup>.

In this presentation the general process as well as mechanism of bioleaching is briefly introduced. In addition, practical work on biofilm development and EPS analysis of bioleaching archaea is also reported.

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## **5.4 Global innovation for value creation in a multinational company**

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Today, innovation is the most important success factor for all enterprises striving for sustainable growth in the chemical industry. The key question herewith is how innovation topics should be defined and resources available are allocated respectively. To catch up with promising innovation topics, megatrends have to be analysed. A megatrend is a big, far-reaching and sustained trend. Alignment to megatrends leads to sustainable growth of the multinational companies and drives innovation in the right direction. "Corporate Foresight" is a dedicated organizational unit of the multinational company which is intensively engaged in the analysis of the megatrends. A multinational company should drive innovation with a global network, balancing short to mid-term innovation and mid to long term innovation. The short to mid-term innovation mainly focuses on existing technologies and markets, and the company works closely together with strategic partners; whilst the mid to long term innovation is often derived from megatrends and requests dedicated resources on the corporate level with special organizational units, "Creavis" for instance. The multinational company uses also "Corporate Venturing" to support the innovation and growth strategy by means of minority investments in high-growth start-up companies and leading funds.



留德华人化学化工学会

**Gesellschaft Chinesischer Chemiker und Chemieingenieure in  
der Bundesrepublik Deutschland e.V. (GCCCD)**

GCCCD, a non-profit Chinese academic organization of chemistry, chemical engineering and related fields, composes of members who have experience of studying and working in Germany. The essential goal of GCCCD is to promote the academic exchange among its members, as well as to promote cooperation between Chinese and German academic and industrial institutions in chemistry and related fields. GCCCD organizes regularly academic meetings and helps its members to participate in various events, e.g. “Chun hui Plan”, “National scholarship for Chinese Ph.D. students of excellence” and “Start-up founding forum” etc.

GCCCD, founded in 1988, is meanwhile part of “Chinese Chemical Society”, “Vereinigung Chinesischer Akademischer und Studentischer Gesellschaften in Deutschland e.V.”, “Federation of Chinese Professional Associations in Europe”. In the past 25 years, plenty of subsidiaries have been founded. Jena, Ulm, Stuttgart, Nordrhein-Westfalen and Berlin-Brandenburg are currently the most active ones among them. Alumni and members of GCCCD are presently playing very important roles in numbers of branches (both in academia and industry, in China and Germany), including many famous scholars, professors and executives.

留德华人化学化工学会是一个由在德国工作学习的华人学者、学生组织成立的非营利性学术组织。学会的宗旨是促进成员之间的学术交流及中德两国之间学术界和工业界的相互合作与交流。学会作为留德学者交流合作的平台，每年定期组织学术会议，同时鼓励和组织会员积极参加各类活动，如“春晖计划”，“国家优秀自费留学生奖学金”和“留学生创业交流会”等。

留德华人化学化工学会最初成立于 1988 年，属于中国化学会海外分会（省级），是中国留德学者学生团体联合会的创始会员，同时是全欧华人专业协会联合会的会员。在过去的 25 年中，学会发展建立了各地的分会组织。目前活跃的分会包括耶拿、乌尔姆、斯图加特、北莱茵威斯特法伦及柏林-布兰登堡分会。留德华人化学化工学会的新老会员们现在活跃在中德两国的学术界和工业界，包括很多知名学者、教授和公司高管。

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### Deutschland Alumni China 中国留德校友 (DACH)

In den letzten zehn Jahren ist die Zahl der Chinesen, die Deutschland als Studien- oder Forschungsort wählten, immer weiter gestiegen. Insofern gibt es auch immer mehr Chinesen, die nach dem Auslandsaufenthalt nach China zurückkehren, um ins Arbeitsleben einzusteigen oder weiterzuarbeiten. Die Erfahrungen, die sie in Deutschland gesammelt haben, werden dabei zu einem wichtigen Grundkapital für ihre weitere berufliche Zukunft. Für viele ist daher der enge Kontakt mit Deutschland und anderen Deutschland-Alumni sehr wichtig.

Unterstützt durch das Bundesministerium für Bildung und Forschung fördert der DAAD dieses Interesse mit der Etablierung und Pflege eines Alumni-Netzwerks für chinesische Deutschland-Alumni. Diesem großen Netzwerk können alle Chinesen beitreten, die länger als drei Monate zum Studium, zur Forschung, zur Weiterbildung oder im Job in Deutschland waren, egal ob der Aufenthalt selbstfinanziert war oder über ein Stipendium. Willkommen in der Familie der Deutschland Alumni China!

近 10 年来, 越来越多的中国人选择到德国学习或研究。也有越来越多的中国人在学业或科研结束以后返回中国开展或者继续他们的事业。在德国的经历成为他们事业成功的重要基石。因此, 很多校友都希望继续同德国及其他留德校友保持联系。

在联邦德国教育与科研部的支持下, DAAD 建立了中国留德校友网络。这一网络面向所有留德国三个月以上的中国人, 无论您是以留学、科研、培训或工作目的赴德, 无论公派、自费或受基金会资助, 都属于我们这一庞大网络。欢迎来到中国留德校友的大家庭中!

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## CENIDE–Center for Nanointegration Duisburg-Essen

The dimension of billionths of a meter is so incredibly small that different physical laws than the familiar world prevail – gold in the nano-dimension is red, iron nanoparticles are so reactive that they ignite themselves. These are just two examples among many. Therefore, nanotechnology offers the possibility to discover new properties in supposedly long-known materials and to use them. The applications of nanotechnology are almost endless and range from power engineering to materials science to medicine.

CENIDE, the “Center for Nanointegration Duisburg-Essen”, represents the appropriate focus of research at the University of Duisburg-Essen (UDE): Since 2005, it links research and teaching activities that deal with the nano-dimension, in natural sciences, engineering and in medicine. In short: CENIDE is the community of nano-researchers at the UDE – the know-how of more than 50 working groups under guidance of designated experts meets here. Partnerships with external members with similar research approaches strengthen the skills spectrum.

One focus of research is nanoenergy – the use of nanotechnology for energy applications. The research building, “NanoEnergieTechnikZentrum, NETZ” opened in February 2013. It is a so far unique complex for the link between basic research and application-related processing for energy technology: In the “linked facilities”, directly interconnected laboratories for engineers, chemists and physicists, nanomaterials will be produced, investigated and processed immediately for energy applications.

As a central scientific institution of the UDE and as a partner of the cluster NanoMikroWerkstoffePhotonik.NRW CENIDE co-determines the projects and goals of nanotechnology research in North-Rhine Westphalia significantly.

### Contact:

CENIDE – Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen

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## Evonik Industries: Core specialty chemicals business

Evonik is one of the world's leading specialty chemicals companies. Profitable growth and sustained value creation form the heart of our strategy. Around 80 percent of sales come from leading market positions, which we plan to expand further. We concentrate on high-growth megatrends, especially health, nutrition, resource efficiency and globalization. Our core specialty chemicals business is divided into three reporting segments:

### Consumer, Health & Nutrition

The segment produces specialty chemicals, principally for applications in the consumer goods, animal nutrition and pharmaceutical sectors.

### Resource Efficiency

The Resource Efficiency segment provides solutions for environment-friendly and energy-efficient products.

### Specialty Materials

The heart of the Specialty Materials segment is the production of polymer materials and their preproducts, and additives.

In 2012 Evonik's roughly 33,000 employees generated sales of €13.6 billion and an operating result (adjusted EBITDA) of €2.6 billion. 75 percent of sales are generated outside Germany, providing convincing evidence that our business is global.

### Exploring opportunities. Growing together.

If you're interested in applying your skills and knowledge to solve the problems of tomorrow, then discover the numerous career opportunities at Evonik Industries and become part of our international team. Learn more about the countless opportunities at Evonik:

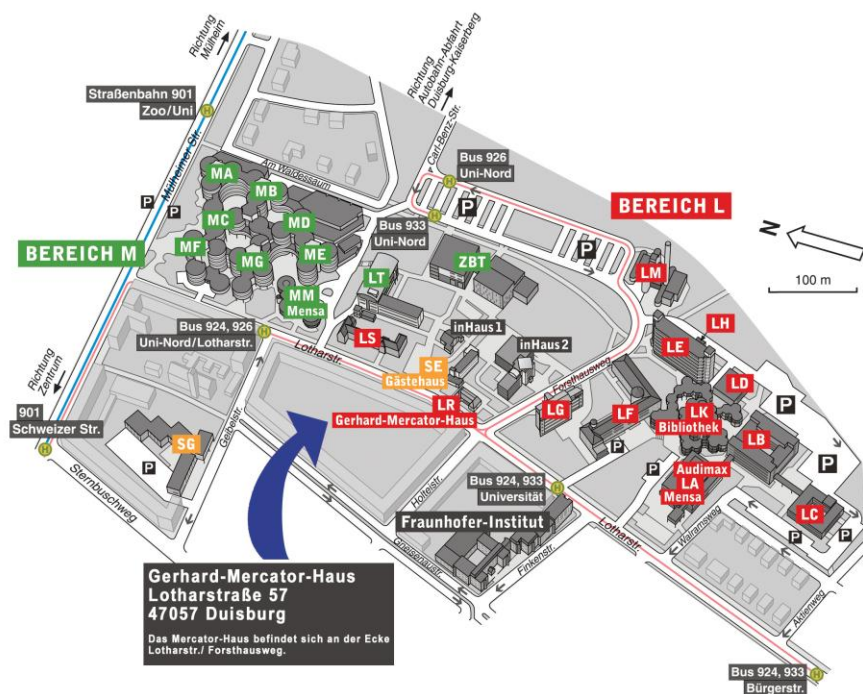




## Travel guide



Conference venue: Gerhard-Mercator-Haus, Lotharstraße 57, 47057 Duisburg



Gerhard-Mercator-Haus (LR) on the Duisburg-campus map of the University of Duisburg-Essen

More information about arrival please read: [http://www.uni-due.de/cenide/anfahrt\\_mercatorhaus.shtml](http://www.uni-due.de/cenide/anfahrt_mercatorhaus.shtml)

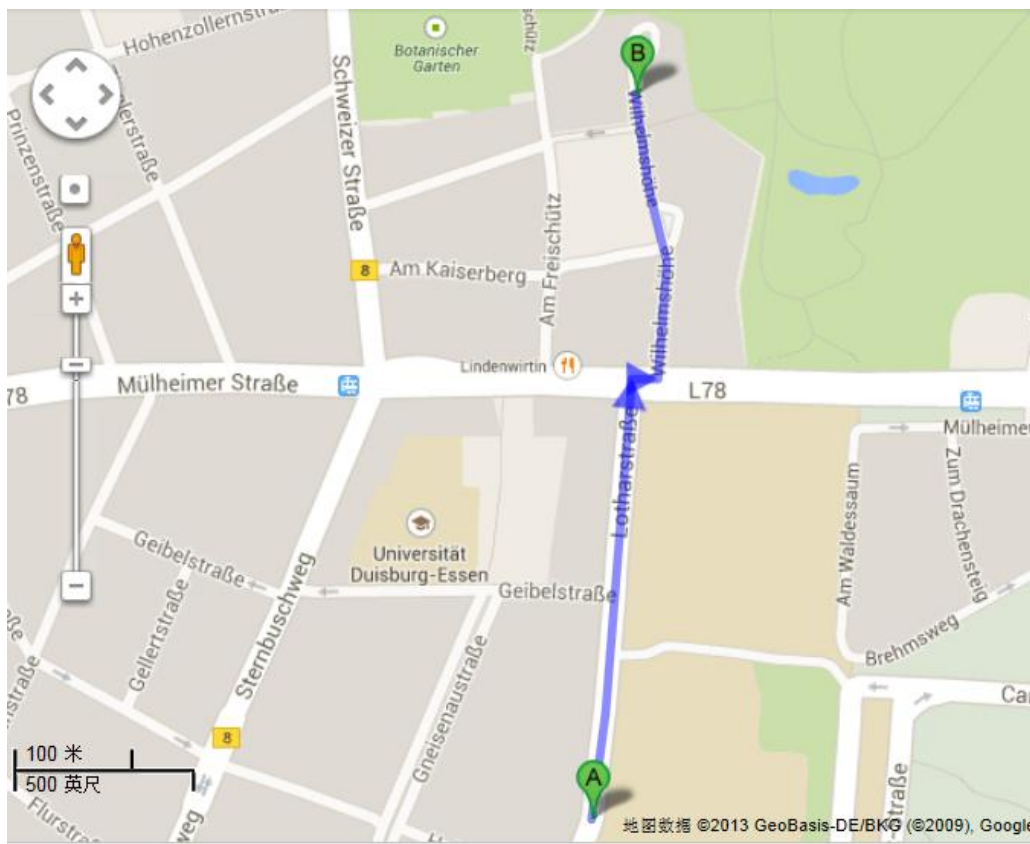


Address of the 25<sup>th</sup> GCCCD Anniversary Banquet:

**Restaurant Kaiserberg Terrassen Wilhelmshöhe  
Am Botanischen Garten 21  
47058 Duisburg**

Entrance starts: 18:30

Official banquet program starts at 19:00 and ends at 22:00.



From Gerhard-Mercator-Haus (A) to Restaurant Kaiserberg Terrassen Wilhelmshöhe (B)  
(10 minutes of walk)

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