## GCCCD 2012 Conference

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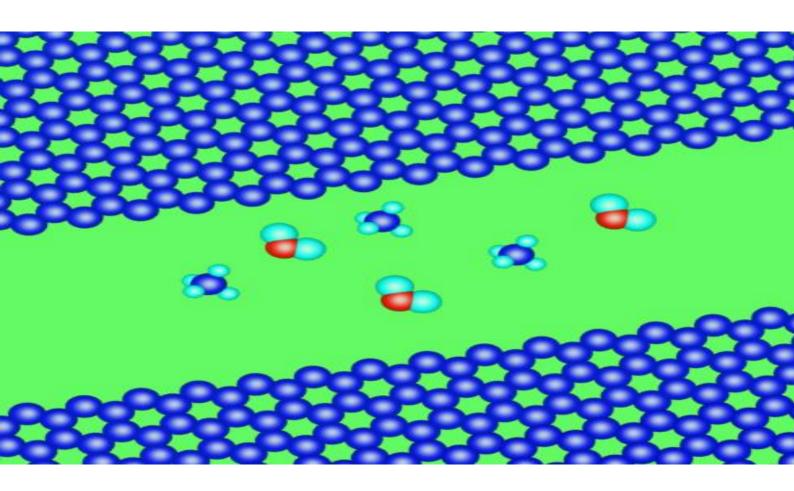
(留德华人化学化工学会第24届年会)



Gesellschaft Chinesischer Chemiker und Chemieingenieure in der Bundesrepublik Deutschland

### October 27th to 28th, 2012

Department of Chemistry Gerhard-Domagk-Str.1, 53121 Bonn









## 中国驻德国使馆教育处

Abteilung für Bildungswesen der Botschaft der Volksrepublik China in der Bundesrepublik Deutschland



Rheinische Fachgruppe Chemie Friedrich-Wilhelms-Universität Bonn



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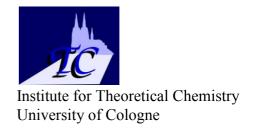


## 中华人民共和国 驻德意志联邦共和国大使馆教育处

Abteilung für Bildungswesen der Botschaft der Volksrepublik China in der Bundesrepublik Deutschland



Rheinische Fachgruppe Chemie Friedrich-Wilhelms-Universität Bonn



### **Acknowledgements**

We greatly appreciate the generous sponsorship from LANXESS, EVONIK, and BASF. We also owe many thanks to the Education Section of the Chinese Embassy in Germany for providing us with long term solid financial support, due to which the continuity of the GCCCD Conference has been guaranteed. The kind support by the Department of Chemistry, University of Bonn, and by the Institute for Theoretical Chemistry, University of Cologne, are deeply acknowledged. We would also like to sincerely appreciate for the generous donations made by several individuals. We are deeply indebted to Dr. Wilfried Assenmacher for the technical support with sacrificing his invaluable weekend. Last but not least, we thank all the participants for sharing their time and expertise.

### **Organisation Committee**

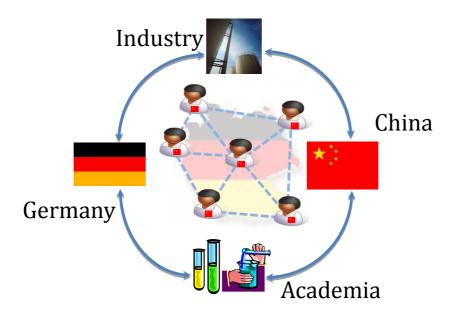
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### **About GCCCD**

GCCCD (Gesellschaft Chinesischer Chemiker und Chemieingenieure in der Bundesrepublik Deutschland) was founded in August 1988. As an academic society of Chinese chemists and chemical engineers in Germany, GCCCD is devoted to promoting academic exchange and establish a network between Chinese chemists and chemical engineers who are working in Germany, as well as to bridge the gap between the Chinese scientists and the German and Chinese academia and industry.



GCCCD is an overseas branch of the Chinese Chemical Society, a member of the "Vereinigung Chinesischer Akademischer und Studentischer Gesellschaften in Deutschland e.V." and the "Federation of Chinese Professional Associations in Europe". In the past few years branches of GCCCD have been founded in the cities Braunschweig, Jena, Ulm and Stuttgart, as well as in the federal states Nordrhein-Westfalen and Berlin-Brandenburg.

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## Program

### 27th October, Saturday

10:00-13:00		Arrival registration (lunch)
13:00-13:20	Section 1-1	Welcoming and Opening Remarks
13:20-14:50	Section 1-2	Chair: Dr. Wei Xia
13:20-13:50	Prof. Michael Dolg	Relativistic Effects in Electronic Structure Calculations for Heavy
Inv. Speaker 1		Element Compounds
13:50-14:10	Dr. Lisong Xiao	A Green Chemical Approach for Highly Water-Soluble and
Speaker 1		Biocompatible Superparamagnetic Magnetite Nanoparticles for
		Enhanced MRI
14:10-14:30	Dr. Lifei Xi	Surface treatment of hematite photoanode for water oxidation
Speaker 2		
14:30-14:50	Mr. Feng Liang	Fast on-site monitoring of gasoline-related compounds at
Speaker 3		contaminated sites using differential mobility spectrometry
14:50-15:10	Dr. Qiang Ju	The bioapplication of multifunctional nanocrystals
Speaker 4		
15:10-15:40		Break
15:40-17:50	Section 1-3	Chair: Dr. Xingxing Chen
15:40-16:10	Prof. Joachim Mayer	New Developments and Applications of Ultrahigh Resolution
Inv. Speak 2		TEMs
16:10-16:30	Dr. Chunlei Wang	High power handling microsupercapacitors based on
Speaker 5		Graphene/CNT composite
16:30-16:50	Ms. Qiao Yu	Power-to-Gas with Direct-Air-Capture
Speaker 6		
16:50-17:10	Dr. Fei Wang	Deciphering the Chemical Bonding in Anionic Thallium Clusters
Speaker 7		
17:10-17:30	Mr. Xuting Huang	Coupling of Josephson Currents in Quantum Hall Bilayers
Speaker 8		
17:30-17:50	Dr. Harjinder S. Bhatti	Innovation @ Evonik
Inv. Speaker 3		

## 28th October, Sunday

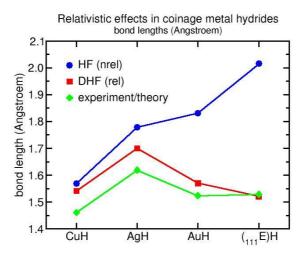
9:10-10:50	Section 2-1	Chair: Dr. Xiaoyan Cao-Dolg
9:10-9:30	Mr. Yanze Ren	Sonoelectrochemical degradation of phenol in aqueous solutions
Speaker 10		
9:30-9:50	Mr. Xiaofeng Wang	Miniaturized Mid-Infrared Sensor Technologies
Speaker 11		
9:50-10:10	Mr. Yunhui Wang	Novel mixed 3-mono-O-alkyl cellulose: Synthesis, structure
Speaker 12		characterization and thermal properties
10:10-10:30	Dr. Shaohua Ju	The Research Progress on Microwave Metallurgical Reactor
Speaker 13		
10:30-10:50	Dr. Rongzhen Liao	Mechanism and Chemoselectivity of Tungsten-dependent Acetylene
Speaker 14		Hydratase, A Quantum Chemical Study
10:50-11:20		Break
11:20-12:50	Section 2-2	Chair: Ms. Lijun Zhang
11:20-11:40	Dr. Cheng Li	Patterning of Functional Nanostructures Using Colloidal Crystals:
Speaker 16		A Bottom-Up Approach
11:40-12:00	Mr. Qingfu Zhu	Capillary Electrophoresis-Based study of Specific activities of
Speaker 17		Methionine Sulfoxide Reductase
12:00-12:20	Dr. Xian Wu	A Super Concentrated History of Chemistry in Germany
Speaker 18		
12:20-12:50 Inv.	LANXESS	
Speaker 4		
12:50-13:50	Lunch	
14:00-16:30	Chemparktour at LAN	XESS

### Relativistic effects in electronic structure calculations

### for heavy element compounds

Michael Dolg Institut für Theoretische Chemie, Universität zu K"oln, Greinstr. 4, 50939 Köln, Germany

Relativistic effects in the electronic structure of atoms and molecules increase with the nuclear charge to the fourth power, i.e., they become more important for the chemistry of heavy elements [1]. A brief overview over the major relativistic effects in atoms (direct and indirect effects leading to orbital contraction/stabilization and expansion/destabilization) as well as molecules (bond length contraction/elongation and bond stabilization/destabilization) will be given. A simple method to include relativistic effects in electronic structure calculations will be described [2]. Finally, characteristic examples, e.g., the inert character of gold, the inert character of the 7s-electron pair in Tl and Pb, the valency of the lanthanides and actinides and the color of gold will be briefly discussed. Finally, it will be explained why (as was recently found) cars start only due to relativity [3].



- [1] P. Pyykkoe, Chem. Rev. 88 (1988) 563-594.
- [2] M. Dolg, X. Cao, Chem. Rev. 112 (2012) 403-480.
- [3] R. Ahuja et al., Phys. Rev. Lett. 106 (2011) 018301.

# A Green Chemical Approach for Highly Water-Soluble and Biocompatible Superparamagnetic Magnetite Nanoparticles for Enhanced MRI

### Lisong Xiao and Sanjay Mathur

Institute of Inorganic Chemistry, University of Cologne, 50354, Cologne.

Ultrasmall superparamagnetic iron oxide nanoparticles (USPIONs) were synthesized by a simple green chemical approach, in which a natural nutrient of vitamin C was used as reducing agent and its oxidized product was further played a role as capping agent. The as-prepared USPIONs have an average core size of 5.1 nm and exhibit good crystallinity and high magnetization saturation value (47 emu.g<sup>-1</sup>). The strong capping effects of oxidized vitamin C on the surface of the particles impart to the USPIONs an excellent solubility and stability in water, PBS buffer and cell culture media, as well as a remarkable biocompatibility as determined using primary human immune-competent cells and the zebra fish embryo tests. Detailed NMR analysis of the suspensions provides insight into the magnetic order within the colloid and demonstrates the suitability of the materials as negative contrast agents for MRI. Phantom experiments on the contrast agent (clinical 3 T MRI scanner) reveal an enhanced  $r_2/r_1$  ratio of 36.4 ( $r_1$ = 5 s<sup>-1</sup>mM<sup>-1</sup> and  $r_2$ = 182 s<sup>-1</sup>mM<sup>-1</sup>) by comparing with the clinically approved SPIOs and USPIOs, which implies the DHAA-Fe<sub>3</sub>O<sub>4</sub> NPs suspensions are expected to be a promising candidate for negative contrast applications. The cellular uptake studies showed that NIH 3T3 cells have much higher uptake of the DHAA-Fe<sub>3</sub>O<sub>4</sub> NPs than Sinerem<sup>@</sup>.

### Surface treatment of hematite photoanode for water oxidation

## Lifei Xi Forschungszentrum Jülich GmbH, Jülich, Germany

Photoelectrochemical (PEC) cells offer the ability to convert solar energy to stored chemical energy through the splitting of water into molecular oxygen and hydrogen. Hematite (a-Fe<sub>2</sub>O<sub>3</sub>) has recently emerged as a promising photoanode material for the generation of dioxygen from water due to its favorable optical band gap (Eg: 2.2eV), excellent chemical stability in aqueous environments, ample abundance and low cost.

In this presentation, I will present few strategies for surface treatment on hematite nanorods for photo-driven water oxidation. It includes spin-coating treatment of zinc acetate on hematite thin film and the growth of Sn treated hematite from α-FeOOH nanorod arrays without substantially altering morphologies. I found that their surface treated samples showed significantly enhanced photocurrents. For example, the photocurrent onset potential of hematite photoanodes was improved by 170 mV after 3 cycles of ZnAc treatment, while the photocurrent was increased from 0.75 to 1.08 mA cm<sup>-2</sup> at 1.23 V vs. RHE. We proposed that the ZnO overlayer changes the flat band potential of hematite and reduces surface defects. Very recently, with Sn treatment the photocurrent density of hematite photoanode increased from 1.24 for pristine hematite nanorods to 2.25 mA/cm<sup>2</sup> at 1.23 V vs RHE (i.e. 81% improvement). The photocurrent density increase is also accompanied by improved incident-photon-to-current efficiencies and oxygen evolution. The photocurrent improvement is mainly attributed to an increase in surface passivation through the formation of Fe<sub>x</sub>Sn<sub>1-x</sub>O<sub>4</sub> layer at the surface as shown by XPS, HRTEM, EDAX line scan analysis and PEC measurements.

Indeed, these studies showed that advantageous surface treatments of hematite can be achieved using safe, inexpensive materials and simple processing techniques.

## Fast on-site monitoring of gasoline-related compounds at contaminated sites using differential mobility spectrometry

## Feng Liang *University of Duisburg Essen*

Gasoline consists of aliphatic hydrocarbons, aromatic hydrocarbons and some oxygenates like methyl tert-butyl ether. Most of the aromatic and oxygenated compounds can result in harmful effect to the environment and public health. Groundwater contamination occurs when gasoline contained storage tank leak out. The classic methodology for analyzing the gasoline related compounds in water is based on lab analysis such as GC coupled with FID or MS detector. However, all standardised laboratory based techniques are time consuming and require sample collection, which limit fast and on field monitor gasoline leaking. To save time and cost, it is very important to develop methods to fast screen on site before lab analysis. Although recent field investigations have shown promising results and a great potential, the number of trials carried out under realistic conditions is relatively limited.

Over the past few decades, ion mobility spectrometry has become a highly attractive tool for various applications due to its high sensitive and fast response to chemicals. This project will develop novel methodology based on differential mobility spectrometry (DMS) for fast analysis of water and soil samples at contaminated sites. Extraction methods will be adopted to overcome existing limitations of applying DMS to aqueous phase samples. We will incorporate all approach into a portable instrument to monitor gasoline contaminated water on site.

### The bioapplication of multifunctional nanocrystals

## Qiang Ju Chemistry and Biochemistry Department, Ruhr University Bochum

Cancer is the second leading cause of death, with millions of newly diagnosed cases worldwide each year. The main reason for this dismal picture is that even with the current state of the art of cancer diagnosis, this disease is usually detected in an advanced stage. Therefore, the most important issue for cancer prevention and therapy should be addressed: fabrication of novel probes for diagnosis of this disease at an earlier stage, and facilitated route to simultaneously kill the tumor. A synergistic combination of nanotechnology and biotechnology can provide unprecedented opportunities for addressing many of the current challenges in cancer diagnosis and therapy. Particularly, multifunctional nanoparticles carrying multiple diagnostic probes and therapies can provide both structural and metabolic information specifically from disease sites, thus leading to significantly improved sensitivity and selectivity for detection and remedy of various human cancers.[1]

Many different types of nanomaterials have been developed to provide contrast in the medical imaging: some of them incorporate an imaging moiety into their design, while others provide contrast as a result of their intrinsic materials properties. However, the well-known imaging modalities have their own advantage and disadvantages in sensitivity, resolution, and detecting depth. Combining multiple imaging modalities in a single nanoparticle can exploit the advantages while improving disadvantages of the individual techniques. Here we want to show some bioapplication of multifunctional nanocrystals

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### **New Developments and Applications of Ultrahigh resolution TEMs**

### Joachim Mayer

Central Facility for Electron Microscopy, RWTH Aachen University, 52074 Aachen, Germany, and Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Research Centre Juelich, D-52425 Juelich, Germany

The introduction of aberration correctors has revolutionized the development of TEM and STEM instrumentation. Only shortly after the development and installation of the first TEM with a corrector for the spherical aberration [1], commercial instruments with aberration correctors are now offered by all major manufacturers. In order to provide a platform for these novel developments and based on the experience with the first aberration corrected TEM [2-4], Research Centre Juelich and RWTH Aachen University have jointly founded the Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (ER-C) [5]. Research at the Ernst Ruska-Centre focuses on the development of new quantitative methods in TEM and on their application in materials science and solid state physics. The lecture will give an insight on the latest instrumental developments and on the most important fields of application, which are nanoelectronics and nanomaterials for energy-related systems.

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- [4] C. L. Jia, K. Urban, Science 303 (2004) 2001.
- [5] http://www.er-c.org

## High power handling microsupercapacitors based on Graphene/CNT composite

Chunlei Wang and Majid Beidaghi
Max Planck Institute for Solid State Research

A novel method for fabricating micro-patterned interdigitated electrodes based on reduced graphene oxide (rGO) and carbon nanotube (CNT) composites for ultra-high power handling micro-supercapacitor application will be presented. The binder-free microelectrodes were developed by combining electrostatic spray deposition (ESD) and photolithography lift-off methods. During the ESD process, GO sheets are readily reduced to rGO. Electrochemical measurements show that the in-plane interdigital design of the microelectrodes is effective in increasing accessibility of electrolyte ions in-between stacked rGO sheets through an electro-activation process. Addition of CNTs results in reduced restacking of rGO sheets and improved energy and power density. The addition of CNT, electrolyte-accessible and binder-free microelectrodes, as well as an interdigitated in-plane design result in a high-frequency response of the microsupercapacitors with resistive-capacitive time constants as low as 4.8 ms. These characteristics suggest that interdigitated rGO-CNT composite electrodes are promising for on-chip energy storage application with high power demands.

### **Power-to-Gas with Direct-Air-Capture**

### Qiao Yu Technical University of Dortmund

The so-called power-to-gas technology<sup>1</sup> has the potential to make an important contribution in the effective utilisation of the surplus electricity generated from renewable resources, such as photovoltaics and wind parks, when supply exceeds demand. The increasing use of renewables in place of fossil-based power sources as a consequence of the "energy turnaround" means that the gap between the nominal and actual generating capacities will result in unnecessary wastage, unless some means of storage is adopted<sup>2</sup>.

In the power-to-gas concept, surplus electricity is used to generate hydrogen via water electrolysis, which is employed to catalytically hydrogenate carbon dioxide to methane, which in turn can be transported and stored in the extensive existing natural gas pipeline and reservoir network.

$$CO_2 + 4 H_2 \rightarrow CH_4 + 2 H_2O$$
  $\Delta_R H = -165 \text{ kJ mol}^{-1}$ 

The modest efficiency of the overall conversion process (electrolysis: ca. 70%; CO<sub>2</sub>-methanisation: ca. 80%; overall power-to-gas: ca. 55%) is ameliorated by the carbon-neutral exploitation of an in-place infrastructure with the potential for storing vast amounts of energy over periods of hours to months.

As a carbon dioxide feedstock one can employ biogas or capture the  $CO_2$  direct from the atmosphere. Compare to obtaining  $CO_2$  from a large point resource, the most significant merit of the direct air capture is avoiding the transportation cost of the  $CO_2$  feedstock, which can utilize the wind bringing the air with  $CO_2$  direct to the site. Hence direct air capture would be one potential way to provide  $CO_2$  resource.

<sup>[1]</sup> T. Trost, S. Horn, M. Jentsch, M. (2012), Erneuerbares Methan: Analyse der CO<sub>2</sub>-Potenziale für Power-to-Gas Anlagen in Deutschland, Z Energiewirtsch 36:p. 173-190, DOI 10.1007/s12398-012-0080-6.

<sup>[2]</sup> G. Kreysa (2012), Presentation: Chemical Engineering Challenges for a post-nuclear and post-fossil energy future, CHISA 2012.

### **Deciphering the Chemical Bonding in Anionic Thallium Clusters**

## Fei Wang Department of Inorganic Solid State Chemistry Max Planck Institute for Solid State Research

Tl clusters are ubiquitous among Tl containing compounds, including intermetallics and oxides. They are well-known for being "hypoelectronic", [1-2] *i.e.* their valence electrons counts are less than those required by Wade-Mingos' rules. Previous reports revealed that spin-orbit coupling (SOC) and Jahn-Teller Distortion (J-T) play important roles in stabilizing these clusters. [4,5] We are hereby conducting retrospective investigations with DFT calculations into several prototypical Tl cluster compounds. Energy and electronic structure analyses upon both extended crystal structures and excised Tl clusters were performed to demonstrate the stabilizing effects of SOC and J-T and to elucidate their mechanisms.

<sup>[1]</sup> Corbett, J. D. Angew. Chem. Int. Ed. 2000, 39, 670.

<sup>[2]</sup> Corbett, J. D. Diverse Naked Clusters of the Heavy Main-Group Elements. Electronic Regularities and Analogies; Structure and Bonding, 1997, 87, 157.

<sup>[3]</sup> Wedig, U.; Saltykov, V.; Nuss, J.; Jansen, M. J. Am. Chem. Soc. 2010, 132, 12458.

<sup>[4]</sup> Saltykov, V.; Nuss, J.; Wedig, U.; Jansen, M. Z. Anorg. Allg. Chem. 2011, 637, 357.

### **Coupling of Josephson Currents in Quantum Hall Bilayers**

## Xuting Huang Max Planck Institute for Solid State Research

We study ring-shaped (Corbino) devices made of bilayer two-dimensional electron gases in the total filling factor one quantized Hall phase, which is considered to be a coherent Bardeen-Cooper-Schrieffer-like state of interlayer excitons. Identical Josephson currents are observed at the two edges while only a negligible conductance between them is found. The maximum Josephson current observed at either edge can be controlled by passing a second interlayer Josephson current at the other edge. Because of the large electric resistance between the two edges, the interaction between them can only be mediated by the neutral interlayer excitonic ground state.

### **Innovation @ Evonik**

## Dr. Harjinder S. Bhatti Evonik Industries AG

Evonik Industries AG is one of the global leading specialty chemicals company with production sides in more than 25 countries worldwide. More than 80 percent of the business is generated in business where Evonik ranks among the market leaders. For profitable growth in the near to midterm future, innovation is essential for Evonik. Within this presentation Evonik Industries is introduced briefly and the overall approach how Evonik deals with R&D and innovation is explained. A special focus is drawn to the importance that corporate foresight, corporate venturing and an modern open innovation approaches will have for the future business development and the creativity and innovativity of the company. New approaches in webbased open innovation will be presented.

### Sonoelectrochemical degradation of phenol in aqueous solutions

### Yanze Ren

Institute for Technical Chemistry and Environmental Chemistry Friedrich-Schiller-University Jena

Increasing demand and shortages of clean water sources are serious issues worldwide due to rapid industrial development, population growth and long-term droughts [1]. Contamination, especially by organic pollutants, of the water supply can occur any-38 where within the water supply system [2]. An important group of organic pollutants are the phenolic compounds. Phenol is a common material and a primary pollutant of various industries. The toxicity of phenol, its high usage/production in industry and its stability in the environment make phenol an important target for water treatment. However; due its stability, the treatment of this pollutant group with traditional disposal methods is difficult.

Sonoelectrochemistry is defined as the field of research dealing with the influence of power ultrasound on electrochemical processes [3]. Sonoelectrochemical remediation has some remarkable advantages over other oxidative processes. For example, it can be used under mild reaction conditions, facilitates excellent mass transfer of reaction solutions, maintains electrode activity during the process and is able to treat toxic pollutants over a wide range of concentrations. This makes the sonoelectrochemical process a safe and effective technology, which uses only electricity as a reactant [4-5]. The sonoelectrochemical degradation of phenol in aqueous solutions with stainless steel electrodes and high-frequency ultrasound (850 kHz) was investigated. A 60% synergetic effect was obtained in the combined reaction system. High concentration of electrolyte (sodium sulfate) and a high electrical voltage are favorable conditions for the degradation of phenol. A nearly complete degradation of phenol was achieved with 4.26 g/L Na2SO4 and 30 V electrical voltages at 25°C in 1 hour. The degradation of phenol follows pseudofirst order kinetics. Considering costs and application, the energy efficiency of the reaction system with different reaction conditions was evaluated.

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### **Miniaturized Mid-Infrared Sensor Technologies**

Xiaofeng Wang <sup>1</sup>, Seong-Soo Kim <sup>1</sup>, Robert Roßbach <sup>2</sup>, Michael Jetter <sup>2</sup>, Peter Michler <sup>2</sup>, and Boris Mizaikoff <sup>1,\*</sup>

<sup>1</sup> Institut für Analytische und Bioanalytische Chemie, Universität Ulm, Deutschland <sup>2</sup> Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Deutschland boris.mizaikoff@uni-ulm.de

Mid-infrared (MIR; 3-20μm) spectroscopy is based on exciting vibrational and rotational modes associated with most organic and inorganic molecules, and provides inherent molecular selectivity particularly attractive for sensing applications. Despite this potential, early applications of MIR spectroscopy were mostly confined to a laboratory environment due to the dimensions of conventional IR-spectroscopic equipment. Considering the prevalent miniaturization/integration of UV-Vis and Near-infrared (NIR) optical devices, the opportunities for miniaturized MIR sensors are evident, in particular for in-situ and on-site monitoring/sensing.

Based on the contributions of our research group [1] toward on-chip IR sensor technology, we will discuss recent progress in miniaturizing such devices utilizing quantum cascade lasers (QCL) [2] in combination with planar GaAs/Al<sub>0.2</sub>Ga<sub>0.8</sub>As waveguides [3]. Aiming at cheap and mass-producible yet sensitive on-chip MIR sensor components, we will furthermore present progress toward structured MIR GaAs/Al<sub>0.2</sub>Ga<sub>0.8</sub>As waveguides based on strip waveguides and microring resonators inspired by the figures-of-merit reported for UV/Vis and NIR resonant cavities [4,5].

The combination of QCLs with microfabricated waveguides aims at single-mode control and enhanced evanescent field intensities for chemical/biological analysis. Based on a previously reported lateral waveguide structure (GaAs/Al<sub>0.2</sub>Ga<sub>0.8</sub>As) [3], thin film planar waveguides were deposited on a GaAs wafer via metal-organic vapor-phase epitaxy (MOVPE). To create strip waveguides and resonators, two different approaches strategies were applied: (a) photolithography combined with reactive ion etching (RIE), and (b) microfabrication based on focused ion beam (FIB) milling. External cavity quantum cascade lasers (EC-QCL) with a wide tuning range of 1570-1735 cm<sup>-1</sup> were combined with such waveguides for studying protein folding within the enhanced evanescent field provided at such novel MIR waveguide architectures. Finite element modeling (FEM) was applied for advanced mode analysis and for studying the beam propagation properties for designing tapered waveguide, directional couplers, and microring resonators toward integrated MIR micro-/nano-optics. Recent studies reveal that molecules may be detected with yet unachieved sensitivity in the MIR by determining e.g., a resonance peak shift, a change in Qfactor, or a refractive index change at the surface of such resonant devices, which paves the way toward future direct and label-free detection of biomolecular interactions using portable MIR sensing systems taking advantage of on-chip fabrication technology.

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## Novel mixed 3-mono-O-alkyl cellulose: Synthesis, structure characterization and thermal properties

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The 3-mono-O-alkyl cellulose samples bearing two different ether moieties, namely methyl/ethyl, methyl/n-propyl, and ethyl/n-propyl were synthesized applying protecting group technique. The NMR spectra of the peracetylated products revealed the regioselectivity of the alkylation as well as the degree of substitution of both alkyl moieties. The number average degree of polymerization ( $DP_n$ ) calculated from size exclusion chromatography decreases from  $DP_n$  117 (starting cellulose, Avicel PH-101) to  $DP_n$  range of 20-50 due to the multi-step synthesis. It could be demonstrated that the lower critical solution temperature (LCST) is influenced by the degree of substitution of both alkyl groups. For example, LCST values between 33 and 58°C were measured for aqueous solutions of 3-mono-O-ethyl/n-propyl cellulose. On the contrary, the thermal behaviour of a physical mixture of 3-mono-O-ethyl- and 3-mono-O-propyl cellulose, e. g., was controlled by the derivative with the lowest LCST.

### 微波反**应**器研究**进**展

### 巨少华

### 昆明理工大学非常规治金教育部重点实验室

清洁生产、节能降耗、绿色制造和循环经济是目前工业领域的时代主题,将微波能这种清洁能源应用到化工、冶金等的高能耗、高污染工序中,充分利用其内部加热、清洁可靠、催化效应和易于控制的特点,是实现上述目标一种重要的手段。目前已经成为工业领域重要的研究热点。我实验室以研究微波与颗粒物料相互作用为指导,针对冶金、化工过程的多样性和复杂性,在解决反应器核心难题、实现微波反应器大型化、连续化和自动化的基础上,进行关键技术开发,将微波能成功应用到了冶金碳热还原、锂离子正极材料烧结、高比表面活性炭制备、强腐蚀溶液清洁加热、冶金废渣脱除氟氯、材料膨化、清洁热风、铀化学品烧结、清洁干燥、助磨、助浸等领域,产生了良好的经济效益和社会效益。

### The Research Progress on Microwave Metallurgical Reactor

#### Shaohua Ju

Key Laboratory of Unconventional Metallurgy, Ministry of Education Kunming University of Science and Technology

Nowadays, cleaner production, energy and material saving, green manufacturing and circular economy are the themes of the times in industry fields. Making full use of the characters of microwave energy such as heating inside, clean, reliable, catalytic effect and easy control, and applying this clean energy into some procedure of high energy consumption, high pollution site, are one of the important ways to realize the above aim. Thus, microwave application is becoming a heated research focus. Based on the theory study of the interaction of microwave with material particles and the diversity and complexity of metallurgy and chemical engineering, our laboratory has solved several key problems for realizing amplification, continuous and automation of microwave reactor. After continuously developing of key technologies, we have applied the microwave energy in the fields of carbon thermal reduction of metal oxides, sintering of Li ion cathode material, preparation of activated carbon with high surface area, clean heating of high corrosion solution, F, Cl chemicals removal from metallurgical dust, materials puffing, clean hot air, sintering of U chemicals, clean dry, grinding aid, leaching aid, et al., which have shown excellent economic benefits and social benefits.

## Mechanism and Chemoselectivity of Tungsten-dependent Acetylene Hydratase, A Quantum Chemical Study

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The tungsten-dependent acetylene hydratase catalyzes the nonredox hydration of acetylene to acetaldehyde.<sup>1</sup> A new reaction mechanism was proposed to explain the unusual reactivity of this enzyme using quantum chemical methods.<sup>2,3</sup> The mechanism involves direct coordination of the acetylene to the tungsten ion, followed by a nucleophilic attack by a water molecule in concomitant with a proton transfer to a second-shell aspartate, which then delivers the proton to the substrate. The suggested mechanism has been further used to rationalize the chemoselectivity of this enzyme, where propyne, ethylene, and acetonitrile cannot be hydrated.<sup>4</sup>

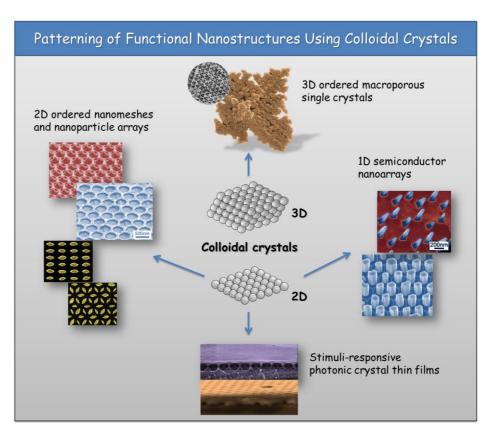
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## Patterning of Functional Nanostructures Using Colloidal Crystals: A Bottom-Up Approach

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### **Graphical abstract:**



 $\textbf{Fig. 1} \ \textbf{Bottom-up fabrication of patterned functional nanostructures using three-ortwo-dimensional colloidal crystals}$ 

#### **References:**

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## Capillary Electrophoresis-Based Study of Methionine Sulfoxide Reductase

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The methionine sulfoxide reductases MsrA and MsrB are repair enzymes that reduce methionine sulfoxide [Met(O)] residues in oxidatively damaged proteins to methionine (Met) residues in a stereospecific manner. These enzymes protect cells from oxidative stress and have been implicated in delaying the aging process and progression of neurodegenerative diseases. Met is one of the most easily oxidized amino acids by reactive oxygen species yielding a mixture of the two epimers because the sulfur in Met(O) is a chiral center. The reduction procedure is catalyzed by either MrsA, which reduces the S epimer of Met(O) [Met-S-(O)], or the MsrB proteins, which reduce the R diastereomer of Met(O) [Met-R-(O)], in proteins in the presence of a reducing system.

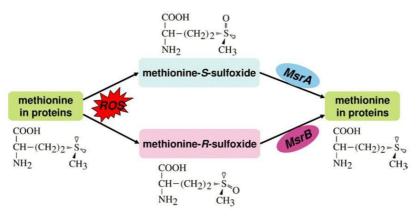


Figure 1 A pathway of methionine sulfoxide reduction

Capillary electrophoresis (CE) has been proven to be a very powerful analytical technique for the analysis of closely related compounds including stereoisomers. In this presentation the use of CE for studying the stereoselective reduction of Met(O) by Msr enzymes is discussed.

A CE method was developed for the analysis of Met(O) diastereomers after derivatization with dabsyl chloride. Separation of the Met(O) diastereomers, Met and  $\beta$ -Ala as internal standard was achieved in 75 mm ID fused-silica capillary coated by a multiple ionic-polymer layer using a background electrolyte composed of 35 mM sodium phosphate buffer, pH 8.0, containing 25mM SDS at 20°C and an applied voltage of 25 kV. Detection was performed at 465 nm. The method was validated and applied to investigate the stereoselective reduction of Met(O) by Msr enzymes from different sources.

### A Super Concentrated History of Chemistry in Germany

### Xian Wu

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化学在作为一门科学被确立之前被称为炼金术,16 - 17世纪的炼金术士主要有两派:亚里士多德学派(主张物质四元素说)和帕拉塞尔苏斯学派(主张物质三要素说)。后者的代表人物帕拉塞尔苏斯(Paracelsus, 1493-1531)生于瑞士,母语为德语,善于用德语而非拉丁语阐述自己的观点,对德语区的影响较大。1661年英国学者罗伯特•波义耳(Robert Boyle, 1627-1691)出版其对话体名著 - 怀疑的化学家(The Sceptical Chymist),标志着化学作为一门科学的诞生。

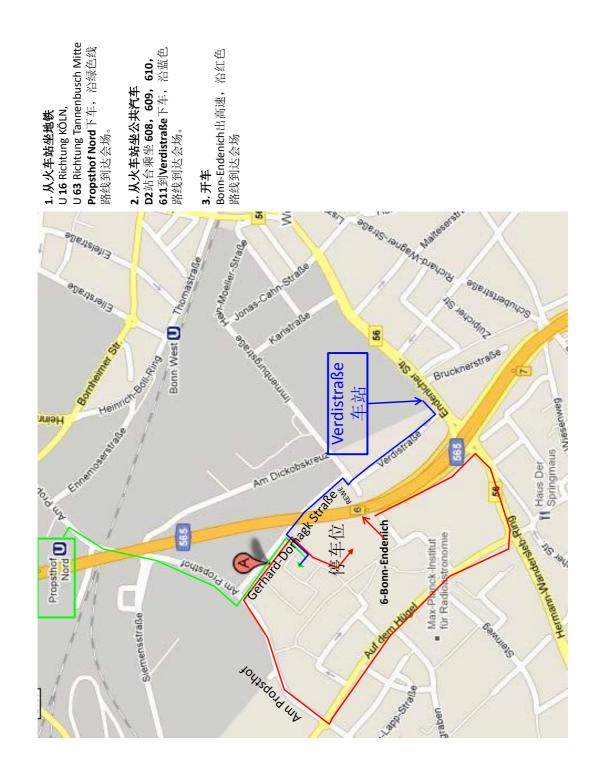
但此后化学并没有迅速发展,而是几乎停滞了一百多年,其原因在于错误的燃素学说主宰当时的化学界。燃素学说最早可以追溯到 1669 年德国学者约翰·约阿西·贝歇尔(Johann Joachim Becher, 1635-1682)出版的土质物理(Physica Subterranea)一书,其中的油状土概念即为燃素的雏形。而真正提出燃素学说的是贝歇尔的学生 - 德国化学家乔治·恩斯特·施塔尔(Georg Ernst Stahl, 1660-1734),他将贝歇尔的油状土概念加以改进和扩充,形成了自己的理论体系,认为存在一种物质叫燃素,是构成火的细小微粒,以游离或化合状态存在,物质燃烧即为释放燃素的过程。该错误理论被当时的大多数化学家所尊崇,直到 18 世纪后期,法国化学家安托-洛朗·拉瓦锡(Antoine-Laurent Lavoisier, 1743-1794)提出正确的氧化理论,才结束了燃素学说在化学界的统治状态,自此化学得以迅速发展。

到了 19 世纪中期,德国化学开始崭露头角,时任吉森大学教授的化学家尤斯图斯•利比希(Justus Liebig, 1803-1873)开创吉森学派,主张化学教育应以实验为重,并建立了第一个化学学生实验室,培养了众多德国和外国重要化学家,而吉森也成为当时的世界化学研究和教学中心。利比希被誉为德国化学之父、有机化学之父和农业化学之父。他与弗里德里希•维勒(Friedrich Wöhler, 1800-1882)和罗伯特•本生(Robert Bunsen, 1811-1899)并称为当时的德国化学三泰斗。

与此同时,德国的有机化学工业兴起,著名化工企业如巴斯夫(BASF)、拜尔(Bayer)、赫希斯特(Höchst)等纷纷成立,有机化工特别是染料工业成为德国经济腾飞的重要产业。物理化学也在威廉·奥斯特瓦尔德(Wilhelm Ostwald, 1853-1932)和雅可布斯·亨里克斯·范特霍夫(Jacobus Henricus van 't Hoff, 1852-1911)的推动下作为化学的一个分支得以确立。德国化学专业协会也在此时应运而生,并创办了若干一直延续至今的重要化学期刊。

从 19 世纪中期到二战结束的将近一百年,德国作为世界化学中心大大促进了 该学科的发展,在化学的历史篇章中留下了辉煌的一页。

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