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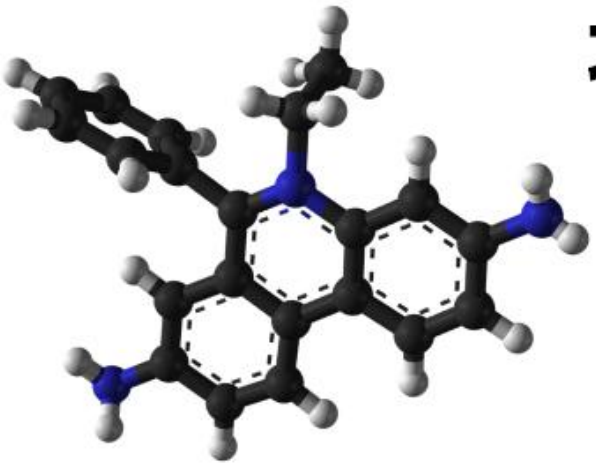

第十届
北威州华人化学化工学术交流年会

10 th Annual Workshop of Chinese Chemists in NRW

29. April 2017

LFI, Hörsaals V, Universitätsklinikum Köln,
Kerpener str. 62, 50937 Köln, Deutschland

主办：

留德华人化学化工学会 西德分会（CGCA-WEST）
波恩-科隆-锡恩地区公派学生学者联合会
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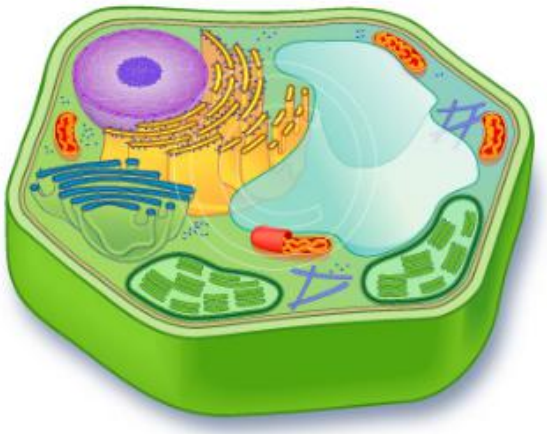

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Organization Committee of the 10th Annual Workshop of Chinese Chemists in NRW held by Chinese-German Chemical Association (CGCA), registered as Gemeinschaft Chinesischer Chemiker und Chemieingenieure in Deutschland e.V. (GCCCD), VR17428, Cologne

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Conference Chair and President of CGCA-West

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University of Wuppertal

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Workshop Program：

09:00-09:30	**Registration**
09:30-10:00	**Opening Remarks**
09:30-09:45	Mr. Dong-sheng Han, Consul in Consulate General of China in Düsseldorf
09:45-09:55 +5 min	Ms. Lin Song, Chair of the 10th Annual Workshop of Chinese Chemists in NRW
10:00-11:30	**Session 1** **Chairwoman: Dr. Xiao-yan Cao-Dolg**
10:00-10:30	*Invited Talk 1: DNA Methylation and Brain Aging* Dr. Xiang-ru Xu, Max-Planck Institute for Biology of Aging, Cologne
10:30-10:50	*Short presentation 1: Application of Metal Organic Frameworks (MOFs) in Photocatalysis* Dr. Yuan-yuan Liu, Institute of Inorganic Chemistry, Heinrich-Heine-University Düsseldorf
10:50-11:10	*Short presentation 2*: *Computations: From Atomic Clusters to Molecular Crystals* Dr. Lei Liu, Max Planck Institute for Polymer Research, Mainz
11:10-11:25 +5 min	**Coffee Break (Poster)**
11:30-12:40	**Session 2** **Chairman: Dr. Xiang-chao Gan**
11:30-12:00	*Invited Talk 2: Transporters of the Multi-Drug-Resistance: Where Biology Meets Chemistry and Physics.* Prof. Dr. Hans-Joachim Galla, Institute for Biochemistry, University of Münster
12:00-12:20	*Short presentation 3: Deletion of the Mas Receptor Aggravates Ang II-Induced Abdominal Aortic Aneurysms Formation in Apolipoprotein-E Knockout Mice* Dr. Guang Yang, Heinrich-Heine-University Düsseldorf
12:20-12:40	*Short presentation 4*: *Comparison of HPV Testing by Real-time Fluorescent PCR and hc2 for Detection of High-grade Cervical Intraepithelial Neoplasia and Cancer: A Case-control Study Among High-risk Patients* Dr. Xin-xin Du, University Hospital of Cologne

12:40-13:45	**Lunch (Poster, Group Photo)**	
13:45-15:40	**Session 3**	**Chairman: Dr. Xiang-ru Xu**
13:45-14:15	*Invited Talk 3: Protein Science Meets Mass Spectrometry: A Perfect Match* Dr. Xin-ping Li, Max-Planck Institute for Biology of Aging, Cologne	
14:15-14:45	*Invited Talk 4: Inter- and Intraspecific Genome Comparison for Trait Diversity* Dr. Xiang-chao Gan, Max-Planck Institute for Plant Breeding Research, Cologne	
14:45-15:05	*Short presentation 5*: *Proton Dynamics in Protein Mass Spectrometry* Mr. Wen-ping Lv, RWTH-Aachen University	
15:05-15:25	*Short presentation 6: IGCC High-temperature Desulfurization over Rare Earth Oxides* Dr. Dong-jing Liu, Rostock University	
15:25-15:40	**Coffee Break (Poster)**	
15:40-17:00	**Forum**	**Chairman: Dr. Yu-jin Tong**
15:40-15:55	*Invited Talk 5: The German Health Care System and Career Prospects for Mediciners* Dr. med. Wei-guo Xu, Krankenhaus Sankt Hubertusstift	
15:55-16:10	*Invited Talk 6: Entrepreneurship and Live in Germany* Ms. M.-Y. Tang, Fujian International Travel Tang (FITT)	
16:10-16:35	Questions and discussions	
16:35-16:45	**Closing Remarks**	
+15 min	Dr. Yu-jin Tong, Chairman of CGCA	

Invited presentation 1

DNA Methylation and Brain Aging

Dr. Xiang-ru Xu; Max Planck Institute for Biology of Ageing, 50931, Cologne, Germany; Yale University School of Medicine, New Haven, CT 06520, USA.

Abstract

Emerging evidence suggests that DNA methylation, an epigenetic mechanism, plays a pivotal role in the pathogenesis of age-related neurological disorders. However, it is still largely unknown how age and favorable age-interventions including dietary restriction (DR) and rapamycin affect the DNA methylation patterns in the brain. By using a cohort of C57/B6 mice with age groups of young (3 months), old (22 months), and old-group matched DR and rapamycin administration, we interrogated DNA methylation pathways, DNA methylation patterns and gene expressions in mouse hippocampal tissues with deep-sequencing approaches. The results showed that DNA methylation pathway decays with mouse hippocampal aging, consonant with a parallel human hippocampal aging study. DR and rapamycin can partially prevent the age-associated deterioration of DNA methyltransferase 1 (Dnmt1) and Dnmt3a2 distinctively. Interestingly, an age-associated redistribution of genome-wide DNA methylation pattern rather than the reduction of overall DNA methylation with aging were observed. CpG methylation rates in the promoter was shown a unique mode and a lower ratio than all other DNA elements regardless of age, and it was remarkably exhibited as the least age-responsive DNA element in terms of DNA methylation. Furthermore, age-related CpG methylation sites and differential methylation regions (DMRs) were identified, and age-related DNA methylation impacts mostly the neuronal gene expression and pathways. Both DR and rapamycin, to some extent, prevent the age-related changes of DNA methylation and gene expression in hippocampus.

Invited presentation 2

Transporters of the Multi-Drug-Resistance: Where Biology Meets Chemistry and Physics.

Prof. Dr. Hans-Joachim Galla; Institute for Biochemistry, Westfälische Wilhelms-Universität Münster, Germany.

Abstract

The central nervous system (CNS) is protected by the blood-brain barrier (BBB), which is mainly composed of capillary endothelial cells connected by narrow tight junctions, which prevent paracellular diffusion of polar molecules. In addition to its protective function, the BBB ensures sufficient nutrient supply of the brain by regulating the transport of endogenous compounds and controlling their selective and specific uptake, efflux and metabolism. A special transport feature is the so-called multi-drug resistance (MDR). ATP depended efflux pumps (ABC-transporters) prevent the treatment of brain diseases by active export of drugs from the brain back into the blood stream.

This research presents new evidence about the expression and the regulation of the activity of different ABC transporters in the brain with special interest on the ABCC3 transporter. This transporter has been expressed in yeast and was reconstituted in proteoliposomes. It will be shown that the ABCC3 acts in a cooperative manner with respect to transport and ATPase activity shining new light on the substrate and inhibitor mediated regulation of this important transporter.

Invited presentation 3

Protein Science Meets Mass Spectrometry: A Perfect Match

Dr. Xin-ping Li; Max Planck Institute for Biology of Ageing, 50931, Cologne, Germany.

Abstract

Mass spectrometry is an analytical technology used to determine the elemental composition of an atom or a molecule. Its development can be dated back to more than one century. This technology had been remained in the field of physics and chemistry for about 80 years. Only in the 1980s, with the development of macromolecule ionization methods, mass spectrometry has only begun to be used in protein science. Proteomics, the study of all proteins present in a biological system, was only realized due to the technological development in mass spectrometry later on.

My talk will take a look back at the history of mass spectrometry, outline the instrumentation and methodology and review the application of mass spectrometry based technology for the qualitative, quantitative and structural analysis of proteome.

Invited presentation 4

Inter- and Intraspecific Genome Comparison for Trait Diversity

Dr. Xiang-chao Gan; Max-Planck Institute for Plant Breeding Research, 50931, Cologne, Germany.

Abstract

A key goal in biology is to understand the genetic basis for phenotypic diversity. High throughput sequencing increasingly enables the detection of genetic differences between individuals but reliable variant calling and identifying causal relationships between genotypic and phenotypic variation remain the key focus for evolutionary biology, human genetics and plant breeding. In this talk, I will report the efforts from my group on variant calling (e.g., software IMR-DENOM) and genome-wide association studies (GWAS). In addition, I will present the reference genome sequence of Cardamine hirsuta, a close relative of the model plant Arabidopsis thaliana with a range of experimental tools available to investigate gene function, and share our experiences on using comparative transcriptomics to identify genome-wide patterns underlying trait diversity between the two species.

Short presentation 1

Application of Metal Organic Frameworks (MOFs) in Photocatalysis

Dr. Yuan-yuan Liu; State key Lab. of crystal, Shandong University; Institute of Inorganic Chemistry, Heinrich-Heine-University Dusseldorf, Germany.

Abstract

MOFs are a new class of crystalline porous materials, consisting of metal ions and organic ligand. MOFs have been widely used in catalysis, gas adsorption and separation etc., due to their large surface area and rich chemical functionality. Some MOFs display semiconductive behavior and photocatalytic activities. We synthesized a MOFs based on Al and terephthalic acid / 2-amino terephthalic acid (Al-TA/Al-ATA), and found that both Al-TA and Al-ATA display photocatalytic O_2 evolution from water. Furthermore, taking the easy coordination of metals ions with amino in Al-ATA, we introduced photoreductive Ni^{2+} into Al-ATA, and obtained Al-ATA-Ni. Al-ATA-Ni displays photocatalytic overall water splitting, producing stoichiometric ratio of 2:1 hydrogen and oxygen. Besides that, we prepared a series of bismuth based MOFs and their photocatalytic properties were investigated. A novel topology structure composed of Bi and trimesic acid (H_3BTC) is synthesized by a solvothermal method. It consists of unique $\{Bi_2O_{14}\}$ unit and two helix chains. The obtained Bi–BTC shows high activity of O_2 production in photocatalysis. Through ion exchange, another structure consisting Bi and BTC (BiO-BTC) is obtained when BiO(HCOO) is used as the starting material. The insertion into the $Bi_2O_2^{2+}$ interlayer cause distortion of the whole structure, which improve the photocatalytic activity. A visible light responsive MOFs based on bismuth and 2-mercapto niacin (denoted as Bi-mna) was synthesized, which also displays efficient photocatalytic activity. Chemical adsorption of CO_2 in a porphyrin based MOFs is realized by introducing Cu^{2+} into the phorphyrin ring, which greatly improve the photocatalytic CO_2 reduction into methanol.

Short presentation 2

Computations: from Atomic Clusters to Molecular Crystals

Dr. Lei Liu; Max Planck Institute for Polymer Research, Mainz, Germany.

Abstract

Density functional theory (DFT) and molecular dynamics (MD) simulations have been used to investigate chemical relevant problems. Topics include:1) electronic structures and chemical bonding situations of isolated atomic clusters. Generally global minimum search techniques are used to find out the most stable structures for given number of atomic clusters. Subsequently, the so-called adaptive natural density partitioning (AdNDP) method is used to analyze their chemical bonding patterns. 2) understanding reaction mechanism for organic reactions via transition state theory and metadynamics simulations. On the one hand, static DFT calculations are performed to find out transitions states and to explore the reaction path. On the other hand, metadynamics simulations are used to sample the whole reaction space and to get the free energy landscape. 3) understanding the reactivity of molecular crystals. In this project, a corrected small basis set Hartree-Fock method (HF-3c) as well as a semi-empirical method (DFTB) are used to study the crystal structures of molecular crystals and their application in hydrogen activation and capture of small molecules.

Short presentation 3

Deletion of the Mas Receptor Aggravates Ang II-Induced Abdominal Aortic Aneurysms Formation in Apolipoprotein-E Knockout Mice

Dr. Guang Yang; Heinrich-Heine University Dusseldorf, Germany.

Abstract

Background: Abdominal aortic aneurysm (AAA) is a degenerative disease characterized by aortic dilation and rupture leading to sudden death. Currently, the only available treatments are open surgery and endovascular repair, and novel therapeutic targets are needed to prevent AAA. Angiotensin (Ang) II-infused apoE-KO mice is often used for AAA study. Ang-(1-7) usually counteracts effects of Ang II by activating Mas receptor. This study investigates the hypothesis that deletion of Mas receptor promotes AngII-induced AAA.

Methods and results: In order to investigate the effects of the Mas receptor on the development of AAA, we used different experimental animal model where we infused Ang II chronically to our apoE-KO or apoE/Mas-KO mice. Mas deficiency increased the incidence of AAA formation significantly compared to apoE-KO mice (apoE-KO 50% vs. apoE/Mas-KO 74%). Consistently, apoE/Mas-KO mice presented a higher aneurysm size, AAA incidence, elastin fragmentation, collagen content, intima-media thickness (IMT), and plasma HDL levels, compared with apoE-KO mice. Blood pressures and cardiac hypertrophy did not differ during chronic infusions of Ang II in apoE-KO and apoE/Mas-KO mice suggesting that Mas deficiency augmented AAA formation seemed to be blood pressure independent. Infiltration of macrophages and T cells were significantly increased in aortas of Ang II treated apoE/Mas-KO mice suggesting an proinflammatory role of the Mas receptor in the development of AAA.

Conclusion: In conclusion, our studies showed that the Mas receptor plays an important role in vascular injury as Mas receptor deficiency aggravates the development of AAA. This was associated with an increase in immune cell infiltration. In particular, we could demonstrate that the Mas receptor is an important factor in macrophage function and deletion of the Mas receptor induces a pro-inflammatory phenotype in macrophages.

Short presentation 4

Comparison of HPV Testing by Real-time Fluorescent PCR and hc2 for Detection of High-grade Cervical Intraepithelial Neoplasia and Cancer: A Case-control Study Among High-Risk Patients

Dr. Xin-xin Du; University Hospital of Cologne, Germany.

Abstract

Introduction: HPV testing is more sensitive than cytology for cervical cancer screening but leads to over referral to colposcopy. This study was designed to compare the diagnostic value of real-time fluorescent polymerase chain reaction HPV detection method with hc2 for high-grade cervical lesions and cancer in order to increase the specificity of HPV testing and facilitate the triage before colposcopy.

Material and Methods: Retrospective analysis the clinical data of 21,550 outpatients receiving cervical cancer screening, real-time PCR and hc2 testing were randomly chosen to test samples. Cervical biopsy under colposcopy was performed to high-risk patients. Histopathology was taken as the diagnostic gold standard. Univariate ANOVA and multivariate logistic regression analysis were adopted.

Results: The sensitivity and positive predictive value was 98.9% and 40.4% of hc2, 93.8% and 42.6% of RT-PCR respectively. Comparing with HPV negative cases, the risk of having HSIL and cervical cancer for 16/18 genotypes positive cases was 8.5 fold-higher (OR=8.48, 95% CI: 4.82~14.92). The risk for other 11 genotypes positive cases was 2.2 fold-higher (OR=2.24, 95% CI: 1.27~3.94). The risk for high-level of viral load group (1×10^5~10^7) was significantly higher than the negative group (OR=1.98, 95% CI: 1.43~2.74).

Conclusion: Real-time fluorescent polymerase chain reaction HPV detection method has better positive predictive value and is useful for triage before colposcopy. Patients with positive HPV 16/18 and high-level of viral load have more risk to develop high-grade cervical lesion and carcinoma and are recommended to undergo colposcopy.

Short presentation 5

Proton Dynamics in Protein Mass Spectrometry

Wen-ping Lv; Computational Biomedicine, Institute for Advanced Simulation IAS-5 and Institute of Neuroscience and Medicine INM-9, Forschungszentrum Jülich, Jülich; Faculty of Mathematics, Computer Science and Natural Sciences, RWTH-Aachen University, 52056 Aachen; Cyprus Institute, Computat Based Sci & Technol Res Ctr, 2121 Aglantzia, Nicosia, Cyprus.

Abstract

Native electrospray ionization/ion mobility-mass spectrometry (ESI/IM-MS) allows an accurate determination of low-resolution structural features of proteins. Yet, the presence of proton dynamics, observed already by us for DNA in the gas phase, and its impact on protein structural determinants, have not been investigated so far. Here, we address this issue by a multi-step simulation strategy on a pharmacologically relevant peptide, the N-terminal residues of amyloidpeptide (A β (1-16)). Our calculations reproduce the experimental maximum charge state from ESI-MS and are also in fair agreement with collision cross section (CCS) data measured here by ESI/IM-MS. Although the main structural features are preserved, subtle conformational changes do take place in the first ~0.1 ms of dynamics. In addition, intramolecular proton dynamics processes occur on the ps-timescale in the gas phase as emerging from quantum mechanics/molecular mechanics (QM/MM) simulations at the B3LYP level of theory. We conclude that proton transfer phenomena do occur frequently during fly time in ESI-MS experiments (typically on the ms timescale). However, the structural changes associated with the process do not significantly affect the structural determinants.

Short presentation 6:

IGCC High-temperature Desulfurization over Rare Earth Oxides

Dr. Dongjing Liu; Rostock University, Germany.

Abstract

Due to its environmental friendliness, economical efficiency, and thermal efficiency, Integrated Gasification Combined Cycle (IGCC) power technology has been regarded as one of the most promising clean coal technologies. However, amounts of toxic H_2S would be produced during the coal gasification process, and thus H_2S removal from coarse coal gas by using solid sorbents plays a key role in IGCC system. Various factors have noticeable effects on the desulfurization performance, such as reaction temperature, textural properties (surface area, pore structures), and feed gas content. A series of cerium-based, lanthanum-based desulfurizers have been synthesized via sol-gel methods and employed for H_2S removal at high temperature in a self-assembled fixed-bed reactor experimental system. The as-prepared desulfurizers have been characterized by using SEM, TEM, BET, XRD, TPR, and XPS to study their micro morphologies, textural properties, phase structures, redox behaviors, and surface elements respectively, the desulfurization kinetics and thermodynamics have also been investigated.

Introduction of CGCA

Chinese-German Chemical Association (CGCA), registered as Gemeinschaft Chinesischer Chemiker und Chemieingenieure in Deutschland e.V. (GCCCD),VR 17428, Cologne, is a non-profit Chinese academic organization of chemistry, chemical engineering and related fields, which composes of members who have experience of studying and working in Germany. The essential goal of CGCA 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. CGCA organizes regularly academic meetings and helps its members to participate in various events, including:

- Organize CGCA Annual Conference in fields of chemistry and chemical engineering, as well as regional academic conferences
- Elect CGCA Young Chemists Awards and declare to Chinese Chemical Society
- Organize and assist members to apply for National Excellent Students Scholarship in Germany
- Post Recruitment information, organize and participate in such activities
- Organize Chunhui Plan, visit domestic institutions in China
- Assist members to apply '100-Plan' and '1000-Plan' projects
- Organizing various chemical and cultural Forum
- Communicate with other chinese societies at universities and professional associations
- Organizing various extracurricular activities, such as visiting companies or institutions, picnic and various sporting activities

CGCA 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. Alumni and members of CGCA 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.

2017 年留德华人化学化工学会西德分会年会报销须知

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