EuroSciCon

DAY 1

Scientific Tracks & Abstracts

European Congress on

Advanced Chemistry

July 12-13, 2018 Paris, France

DAY 1

July 12, 2018

Sessions

Analytical Chemistry | Medicinal Chemistry | Petro Chemicals | Inorganic Chemistry | Environmental Chemistry | Materials Chemistry

Session Chair
Wei Li
University of Tennessee, USA

Session Introduction

Title: **Direct non-oxidative conversion of shale gas to chemicals: selective activation, catalyst regeneration and process intensification**
Jianli (John) Hu, West Virginia University, USA

Title: **Plasma-catalytic hybrid process for CO_2 methanation over Ni/CeZr based catalysts**
Patrick Da Costa, University Pierre et Marie Curie, France

Title: **Computer-aided drug design of selective histone deacetylase inhibitors**
Katarina Nikolic, University of Belgrade, Serbia

Title: **One minute-liquid chromatography of intact proteins**
Xindu Geng, Northwest University, China

Title: **First-principles materials by design for thermodynamically stable low-dimensional electrides**
Mina Yoon, University of Tennessee, USA

Title: **Addressing the opioid crisis by developing analgesic drugs with novel modes of action**
Sylvie Ducki, Universite Clermont Auvergne, France

Title: **Chemistry of phosphinidene intermediates and their applications**
Arif Ali Khan, Guru Gobind Singh Indraprastha University, India

Title: **Physicochemical and rheological properties of whey protein microencapsulated 3, 3'-diindolylmethane**
Abbas Khan, Jilin University, China

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Jianli (John) Hu, J Org Inorg Chem 2018, Volume: 4
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DIRECT NON-OXIDATIVE CONVERSION OF SHALE GAS TO CHEMICALS: SELECTIVE ACTIVATION, CATALYST REGENERATION AND PROCESS INTENSIFICATION

Jianli (John) Hu

Center for Innovation in Gas Research and Utilization, West Virginia University, USA

In the United States and rest of the world, there are abundant shale gas resources which are either physically or economically stranded. Commercially, natural gas conversion to chemicals is based on an indirect conversion route via syngas, followed by subsequent conversion processes (methanol plus metholine to gasoline (MTG) process, or Fischer-Tropsch and product refining). The indirect conversion processes are very capital intensive and less energy efficient. This presentation emphasizes the direct conversion of natural gas constituents (C_1-C_3) into aromatics and olefins using transition metal promoted Zeolite Socony Mobil–5 (ZSM-5) catalysts. Catalyst activity, selectivity, deactivation and regeneration of metal-promoted ZSM-5 zeolite catalysts will be discussed. We will introduce a new approach that employs non-thermal plasma to intensify catalytic reaction for natural gas conversion. Under low reaction severity, this approach synergistically integrates plasma reaction chemistry with novel heterogeneous catalysis that decouples methane activation from catalytic surface reaction, shifting rate-determining step from methane activation (cracking C-H bond) to surface C-C formation. One of the focus areas of the research is to elucidate deactivation mechanism of Ga-Pt prompted HZSM-5 and investigate feasibility of regenerating deactivated catalysts for commercial viability. The variation in daily production volume and the change in shale gas composition over time are hurdles to the engineering design of large chemical plants using shale gas as feedstock. The process intensified modular production at natural gas production site overcomes the hurdles with low capital requirements and flexible deployment and operation. Most importantly, the process intensification reduces energy consumption, waste production, and ultimately resulting in cheaper and sustainable technologies. This presentation includes direct natural gas conversion to aromatics using low-temperature plasma catalytic rector, natural gas pyrolysis for the production of CO_2-free H_2 and carbon nanotubes. The challenge in advance the fundamental science aspects presented in direct natural gas conversion will be discussed.

Biography

Jianli (John) Hu, an experienced Scientist and Engineer, is a Chair Professor and the Director of Center for Innovation in Gas Research and Utilization at West Virginia University. As a Director, he leads the creation of an interdisciplinary research center related to natural gas utilization, which is a strategic area of investment for WVU. He worked as a Director of Technology Innovation at Koch Industries, where he was responsible for developing future technological growth areas related to petrochemicals and catalytic and biological processing. He worked as a Research Manager at Pacific Northwest National Laboratory, undertaking DOE, DOD, and NASA projects. In the late 1990s, he served as a Lead Refinery Engineer for BP Oil. He has been granted 25 U S patents and published more than 90 peer reviewed journal and conference papers.

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PLASMA-CATALYTIC HYBRID PROCESS FOR CO_2 METHANATION OVER NI/CEZR BASED CATALYSTS

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The future regulations in greenhouse gases emissions lead the society to find efficient processes for the stabilization of atmospheric CO_2. Among the different processes, such as reutilization as an alternative to its geological storage, the catalytic valorization of CO_2 methanation, i.e. CO_2 hydrogenation, stands as a promising and industrial-scale applicable technology. Although CO_2 conversion into methane is exothermic and thermodynamically favorable at ambient temperature, a catalyst and high temperatures (> 350°C) are needed in order to achieve acceptable methane yield. Though many different metals have been used to catalyze the methanation process, the catalysts mostly based on Group VIII metals, such as Ni and Ru mainly supported on porous supports, are the most developed catalytic systems. Ni-based catalysts have been widely investigated, because of their good compromise between activity and economics. In order to decrease the operating temperature for the methanation of CO_2, the association of a catalyst with non-thermal plasma have been recently proposed, with dielectric-barrier discharge plasma (DBD), producing a wide variety of active species such as electrons, ions and radicals, improving the CO/CO_2 methanation reaction. In this study, we evaluated the coupled plasma DBD – $Ni/CeZrO_2$ system in studying more particularly, the influence of plasma and other operating parameters.

Biography

B P Da Costa has completed his PhD from University Pierre et Marie Curie and Post-doctoral studies from UC Berkekey. He is now Full Professor at Sorbonne University, in Faculty of Science and Engineering. He has published more than 150 papers in reputed journals and has been serving as an Editorial Board Member of different journals in Chemistry and Chemical Engineering.

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COMPUTER-AIDED DRUG DESIGN OF SELECTIVE HISTONE DEACETYLASE INHIBITORS

Katarina Nikolic[1], Dusan Ruzic[1], Nemanja Djokovic[1], Milos Petkovic[1], Danica Agbaba[1], Maija Lahtela-Kakkonen[2] and A Ganesan[3]

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[2]University of Eastern Finland, Finland
[3]University of East Anglia, Norwich, United Kingdom

The concept of gene expression is continuously explained with epigenetic modification. Post-translational histone acetylation and DNA methylation are dominant epigenetic alterations of the genome. Histone deacetylases (HDAC) play essential role in this process and therefore are very intensively investigated drug targets. The alteration in the structure and function of HDAC isoforms are identified in the pathogenesis of inflammation, cancer, and neurodegeneration. Eleven human HDAC isoforms are sharing a highly conserved catalytic domain. Among them, HDAC6 and SIRT2 are important for a wide range of diseases, due to their unique physiological functions. In our research, we have applied pharmacophore modelling, virtual screening, molecular docking and molecular dynamic methodologies for design and identification of selective HDAC6 and SIRT2 inhibitors. Recently resolved the crystal structure of catalytic domain II of human HDAC6 discovered a wide binding site essential for the substrate recognition. We have successfully used these structural features of human HDAC6 catalytic domain II to rationally design selective HDAC6 inhibitors. Newly published X-ray structures of selective ligand-SIRT2 complexes have revealed high conformational flexibility of this enzyme, and gave us more details about mechanism of action of sirtuin 2 inhibitors. Based on these findings we have performed molecular dynamic study of SIRT2 and tried to explain the conformational changes during enzyme catalysis. Since small number of selective HDAC modulators have been reported so far, rational design of HDAC6 and SIRT2 inhibitors are essential for further progress in discovery of epigenetic drugs.

Biography

Katarina Nikolic has completed her PhD from Faculty of Pharmacy, University of Belgrade. She is an Associate Professor at Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Belgrade, Serbia. The main areas of her research involve: Molecular Modeling, Pharmacophore Modeling, Virtual Screening, Molecular Docking and Molecular Dynamic, Computer-aided Drug Design, Lead Optimisation, Synthesis, and Chemometry. Her research is currently focused on Discovery of Novel CNS Drugs and Antineoplastic Agents. Her team has long-lasting research collaboration with several leading European Universities via few Horison2020/COST projects which are focused on rational drug design and discovery. She has published more than 75 papers in reputed journals.

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ONE MINUTE-LIQUID CHROMATOGRAPHY OF INTACT PROTEINS

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The purpose of the presentation is to develop a new and universe technology for protein analysis in one minute by HPLC, called as one minute-liquid chromatography (OMLC). OMLC includes: (1) the theoretical basis of two variables of substance retention under gradient elution in liquid chromatography; (2) methodology of integrating all assisted operations for substance separation together by online manner in liquid chromatography (LC); (3) a kind of special column whose length is smaller than its inner diameter, called as chromatographic cake (CCK), to be employed for separation unit; (4) several examples for ultra-separation of proteins, peptides , and common small solutes to be tested by reversed phase liquid chromatography, hydrophobic interaction chromatography, ion-exchange chromatography, resulting in successfully complete five separation less in 10 min.

Biography

Xindu Geng graduated from Northwest University (NWU, Xi'an) and became a Faculty Member of Department of Chemistry of NWU, and then a Faculty Member of University of Minnesota in 1982~1983; Visiting Professor of Purdue University separately at Department of Biochemistry in 1982~1984 and at Department of Chemistry in 1995~1996, as well a Visiting Professor of Chemistry Department of Creighton University in 2001. He is the Director of Institute of Modern Separation Science of Northwest University. He has published more than 300 papers in reputed journals, four books, and thus won 2 awards in National Scientific and Technology Rank of China; 5 awards in first rank of Provincial and States in China.

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FIRST-PRINCIPLES MATERIALS BY DESIGN FOR THERMODYNAMICALLY STABLE LOW-DIMENSIONAL ELECTRIDES

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Two-dimensional (2D) electrides, emerging as a new type of layered material whose electrons are confined in interlayer spaces instead of at atomic proximities, are receiving interest for their high performance in various (opto) electronics and catalytic applications. A realization of electrides containing anionic electrons has been a great challenge because of their thermodynamic stability. For example, experimentally, only a couple of layered nitrides and carbides have been identified as 2D electrides. We developed a material by design scheme and applied it to the computational exploration of new low-dimensional electrides. Our approach here offers an important alternative that overcomes the current limitation on discovery of new 2D inorganic electrides. By combining the global structure optimization method and first-principles calculations, we identified new thermodynamically stable electrides that are experimentally accessible. Most remarkably, we, for the first time, reveal an effective design rule for 2D electrides. We then discover another new class of electrides, the first electride with nontrivial band topology, based on 1D building block by coupling materials database searches and first-principles-calculations-based analysis. This new class of electrides, composed of 1D nanorod building blocks, has crystal structures that mimic β-$TiCl_3$ with the position of anions and cations exchanged. Unlike the weakly coupled nanorods of β-$TiCl_3$, Cs_3O and Ba_3N retain 1D anionic electron along the hollow inter-rod sites; additionally, strong inter-rod interaction in C_3O and Ba_3N induces band inversion in a 2D superatomic triangular lattice, resulting in Dirac nodal lines. Our work represents an important scientific advancement over previous knowledge of realizing electrides in terms of both materials and design principles, and should interest the communities of catalytic chemistry, surface physics, and structural chemistry, as well as the related engineering disciplines.

Biography

Mina Yoon has received her PhD degree in Theoretical Condensed Matter Physics from Michigan State University. She is a Research Scientist at ORNL and a joint Professor of Physics at UTK. She is a recipient of a Max Planck Fellowship and the Lee Hsun Young Scientist Award from the Institute of Metal Research, Chinese Academy of Science. She has published more than 75 journal papers and has been serving as an Editorial Board Members of international journals and organizer of various international conferences/workshops.

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ADDRESSING THE OPIOID CRISIS BY DEVELOPING ANALGESIC DRUGS WITH NOVEL MODES OF ACTION

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Chronic pain affects 1.5 billion people worldwide, causing a great deal of discomfort among patients and an enormous economic and societal burden. Inadequate pain control, undesirable side-effects associated with current analgesics as well the recent opioid crisis have revived interest in analgesic drug development. The challenge is to develop original analgesics with novel modes of action to address the unmet needs of patients. Pichon recently reported that disrupting the interaction between the PDZ-containing protein PSD-95, and the endogenous ligand 5-HT2A receptor, reduced hyperalgesia suggesting inhibition of this PDZ protein could result in analgesia. Devilliers reported that TWIK-Related K^+ channel TREK-1 -/- mice were more sensitive than wild-type TREK-1 +/+ mice to painful stimuli, suggesting that activation of TREK-1 could result in pain inhibition. Various approaches of drug discovery were explored in order to develop original analgesic drugs targeting PSD-95 and TREK-1.

Biography

Sylvie Ducki has completed her PhD from the University of Manchester (UK) and Postdoctoral studies at the Arizona State University (USA). She joined the University of Salford for a 6-year lectureship and has been a Professor in Organic and Medicinal Chemistry at Sigma Clermont (France) for 11 years. She has published more than 60 papers in reputed journals and has been serving as an Editorial Board Member of various journals including Anti-Cancer Agents in Medicinal Chemistry, Current Chemical Biology, Medicinal Chemistry.

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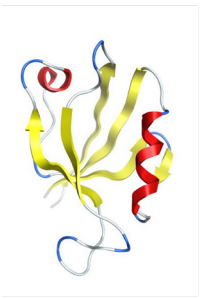
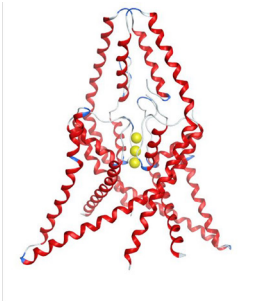


PSD-95

PAIN



TREK-1

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CHEMISTRY OF PHOSPHINIDENE INTERMEDIATES AND THEIR APPLICATIONS

Arif Ali Khan

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Phosphinidene tungsten pentacarbonyl complexes are extremely unstable, highly reactive and could be generated *in-situ* only. These intermediates could be trapped easily in presence of various reagents containing π-systems to afford a number of P-heterocycles. A number of compounds are known to give phosphinidene intermediates but 2H-azaphosphirene tungsten pentacarbonyl complex is the most stable precursor for the *in-situ* generation of terminal phosphinidene complexes. Recently, we found that terminal phosphinidene tungsten pentacarbonyl complex reacted efficiently with the reagents containing no π-systems. For example, a reaction of terminal phosphinidene complex with CCl_4 resulted in dehalogenation, which established the route for the selective insertion of posphinidene complex into carbon-halogen bonds. Such reaction also resulted in dehydroiodination. A reaction of triethylamine with phosphinidene complexes resulted in the formation of primary phosphine complex via dehydrogenation.

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2. A Ozbolat, A A Khan, G von Frantzius, M Nieger and R Streubel (2007) Dehydroiodination of iodo- and diiodomethane by a transient phosphinidene complex. Angew. Chem., Int. Ed. Engl, 46, 2104.

Biography

Arif Ali Khan has recieved his PhD degree in Chemistry from A M U, Aligarh (India) in 1994. Since then he has gained experience as Research Associate and Senior Research Associate at IIT-Delhi and as a Post-doctoral Fellow at Technical University of Braunschweig, Germany. He joined as Lecturer in Chemistry at GGSIP University, New Delhi in 2005. His research interests are in the area of Coordination Chemistry, Organophosphorus Chemistry, Organometallic Chemistry, Metal Ion Catalysed/Promoted Organic Synthesis and Synthesis of Biofuels/ Biodiesel. He has published several research papers in reputed journals. He has successfully completed a number of national projects and international research projects.

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