magnus Group

SEP 13 TO 15 2018

2nd Edition of
Global Conference on

CATALYSIS,
CHEMICAL ENGINEERING & TECHNOLOGY

Theme: Accentuate innovations and emerging novel research in catalysis and chemical engineering

CAT 2018

Exhibitors

micromeritics®
The Science and Technology of Small Particles™

BioLogic
Science Instruments

Publishing Partner

catalysts
an Open Access Journal by MDPI

@catalysis10

VENUE

Holiday Inn Rome Aurelia
Via Aurelia, Km 8.400, 00165
Rome, Italy

http://catalysisevents.com/

Aida Rudakova
Saint-Petersburg State
University
Russia

Akiyo Ozawa
Osaka City University
Japan

Alexander Dennis James
University of Leeds
United Kingdom

Alexandra Mocanu
University Politehnica of
Bucharest, Romania

Amine Bourouina
Laboratoire de Genie des
Procédés Catalytiques, France

Anca Duta Transilvania
University of Brasov
Romania

Andraž Šuligoj
University of Ljubljana
Slovenia

Andrey O. Kuzmin
Boreskov Institute of Catalysis
SB RAS, Russia

Antonyshyn Iryna
Max-Planck-Institut für Chemische Physik fester Stoffe
Germany

Asmaa Bilal Jrad
American University of Beirut
Lebanon

Ayse Hazal Pekcan Cetin
Bogazici University
Turkey

Boris L. Moroz
G.K. Boreskov Institute of
Catalysis, Russia

Borislav Zhivkov Barbov
Institute of Mineralogy and
Crystallography, Bulgarian
Academy of Sciences, Bulgaria

Bruno Azambre
University of Lorraine
France

Byeong-Kyu Lee
University of Ulsan
Republic of Korea

Changhyun Roh
Korea Atomic Energy Research
Institute (KAERI)
Republic of Korea

Choong Kil Seo
Howon University
Republic of Korea

Christophe LEN
Chimie ParisTech
France

Chukhajian Emma H
National Academy of Sciences
Republic of Armenia

Dana Perniu
Transilvania University of
Brasov, Romania

Deliana Dahnum
Korea Institute of Science and
Technology, Republic of Korea

Dietmar Andreas Lang
Disruptive Biotechnology &
Biosourcing, Unilever R&D, UK

Dmitri Gelman
The Hebrew University
Israel

Andrea Zappavigna
Micromeritics SRL
Italy

Jae Young Park
Korea Institute of Industrial
Technology
Republic of Korea

Edoardo Magnone
Dongguk University
Republic of Korea

Efrain Urrutia Bañuelos
Universidad de Sonora
Mexico

Elena Zdravkova Ivanova
Bulgarian Academy of
Sciences, Bulgaria

Eneritz Fernandez-Puertas
GlaxoSmithKline
United Kingdom

Gisela Sabater Pujadas
Shell Global Solutions International, Netherlands

Gwladys Pourceau
University of Picardie Jules
Verne, France

Hans O. A. Fredriksson
Syngaschem BV
The Netherlands

Helmut Schwarz
Technische Universität Berlin
Germany

Hideyuki Okumura
Kyoto University
Japan

Hiroki Sonokawa
Niigata University
Japan

Iris Cornet
Antwerp University
Belgium

Isao Hasegawa
Kansai University
Japan

Ivantsov Mikhail Ivanovich
A .V. Topchiev Institute of
Petrochemical Synthesis,
RAS Russian Federation

Izabela Georgieva Genova
Institute of Organic Chemistry
with Centre of
Phytochemistry, BAS Bulgaria

James J. Spivey
Louisiana State University
USA

Jan Cermak
J. E. Purkinje University
Czech Republic

Jan Schütz
DSM Nutritional Products
Switzerland

Javier Fernandez-Garcia
University of Leeds
United Kingdom

Muhammad Imran Yaqub
SABIC
Saudi Arabia

Jong-Hyun Lee Seoul
National University of Science
and Technology
Republic of Korea

Juha Lehtonen
VTT Technical Research Centre of Finland Ltd, Finland

Jung Hoon Park
Dongguk University
Republic of Korea

Kathrin Maria Aziz-Lange
Helmholtz-Zentrum Berlin für
Materialien und Energie
Germany

Keiji Takata
Kansai University
Japan

Kirill M. Bulanin
Saint-Petersburg State
University, Russia

Kulikova Maya Valer’evna
A. V. Topchiev Institute of Petrochemical Synthesis, RAS
Russian Federation

Kun-Yauh Shih
National Pingtung University
Taiwan

Linga Reddy Enakonda
King Abdullah University
of Science and Technology
(KAUST), Saudi Arabia

Luboš Jankovič
Institute of Inorganic Chemistry, SAS Slovakia

Luis Sánchez Granados
Universidad de Córdoba
Spain

Luisa María Gómez Sainero
Universidad Autónoma de
Madrid, Spain

Mal-Soon Lee
Pacific Northwest National
Laboratory, USA

Pascal Granger
University of Lille
France

Marco Paulo Gomes Sousa Lucas
Universidade de Trás-os-Montes e Alto Douro, Portugal

Maria Armiento
Ford Research and Innovation
Center Aachen, Germany

Maria Chiara Spadaro
Swansea University
UK

Maria Covei
Transilvania University of
Brasov, Romania

María Martín Martínez
Universidad Autónoma de
Madrid, Spain

Masayuki Yagi
Niigata University
Japan

Michalina Stawowy
Wrocław University of Science
and Technology, Poland

Mihail Yordanov Mihaylov
Bulgarian Academy of
Sciences, Bulgaria

Mohammad Naseem Akhtar
King Fahd University of Petroleum
& Minerals, Saudi Arabia

Montserrat Rodriguez Delgado
University of the Balearic
Islands, Spain

Moo Whan Shin
Yonsei University
Republic of Korea

Myriam Frey
LGPC (Lyon)
France

Navid Saeidi
Helmholtz Center for Environmental Research-UFZ
Germany

Nikola Biliškov Ruđer
Bošković Institute
Croatia

Oleg Levin
St. Petersburg State University
Russian Federation

Osamu Tomita
Kyoto University
Japan

Orazio Russo
Micromeritics SRL
Italy

Pascal Fongarland
University of Lyon 1- LGPC
France

Q. B. Broxterman
InnoSyn B V
The Netherlands

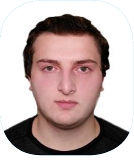
Radostina Nikoaleva Ivanova
Bulgarian Academy of Science
Bulgaria

Rasha Mohamed El Nashar
Cairo University
Egypt

Reza Vakili
The University of Manchester
UK

Richard E. Palmer
Swansea University
UK

S.V. Prabhakar Vattikuti
Yeungnam University
Republic of Korea



Zviadi Zarkua
Tbilisi State University
Tbilisi Georgia

Sanja Panic
University of Novi Sad
Serbia

Serge Cosnier
Grenoble
Alpes University, France

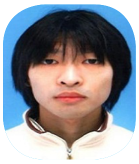
Shun Nishimura
Japan Advanced Institute of
Science and Technology
Japan

Shunsuke Watabe
Niigata University
Japan

Siang-Piao Chai
Monash University
Malaysia

Sorood Zahedi Abghari
Research Institute of
Petroleum
Industry (RIPI), Iran

Stanislaw Dzwigaj
Sorbonne Universités
France



Tetsuya Sato
Niigata University
Japan

Tomoko Yoshida
Osaka City University
Japan

Totka Todorova
Bulgarian Academy of
Sciences, Bulgaria

Valérie Meille
University of Lyon
France

Verziu Marian Nicolae
Institute of Organic Chemistry
'C. D. Nenitescu' of Romanian
Academy, Romania

Victor Zamakhaev
Terratec LLC
Russian Federation

Vinh Q. Mai
National University of Ireland
Galway, Ireland

Virginija Kepenienė
Center for Physical Sciences
and Technology, Lithuania

Vladimir Tsemakhovich
Tel Aviv University
Israel

Volha Matylitskaya
Vorarlberg University of
Applied Sciences, Austria

Wlodzimierz Tylus
Wroclaw University of Science
and Technology, Poland

Yaxin Su
Donghua University
China

Yongha Oh
RSP
Republic of Korea

Yuma Kato
Osaka City University
Japan

Yuuki Tanahashi
Niigata University
Japan

Zhonghua (John) Zhu
The University of Queensland
Australia

Aigerim Baimyrza
Nazarbayev University
Kazakhstan

Ayşe Neren Ökte
Boğaziçi University
Turkey

Bruno Zelić
University of Zagreb
Croatia

Christo Boyanov Boyadjiev
Bulgarian Academy of
Sciences, Bulgaria

Duygu Tuncel
Boğaziçi University
Turkey

Gulzat Demeuova
Nazarbayev University
Kazakhstan

Halit Cavusoglu
Selcuk University
Turkey

Hohyeong Kim
Korea Institute of Industrial
Technology
Republic of Korea

Mikhalenko Irina Ivanovna
RUDN University
Russia

Muhammad Suleman
Jiangsu University
China

Vladimir Ivanovich Parfenyuk
Institute of Solution Chemistry
of the Russian Academy of
Sciences, Russia

Sébastien Tilloy
University of Artois, CNRS,
UCCS
France

Tetiana Kulik Chuiko
Institute of Surface Chemistry
NASU
Ukraine

Alberto Gasparotto
Padova University
Italy

Welcome Message

Dear all attendees, I am extremely proud and feel privileged to write a few welcome notes for the prestigious conference « Catalysis, Chemical Engineering and Technology » – CAT 2018 helded in Rome, the historic city that had an huge impact on civilization. This event dedicated to catalysis will provide a highly interactive platform for relevant experts from the academic and industrial areas to exchange education and research face to face. Chemists and chemical engineers have the means to pave the way to a more widespread implementation of catalysis strategies for the creation of novel catalytic reactions as well as production of industrially relevant products in the future. Importantly, I hope that all the demonstrated advantages of catalysis can stimulate further advances in the field from the younger generations for the benefit of the chemical industry.

Christophe LEN
Chimie ParisTech
France

Welcome Message

Dear conference visitors, it is an honor and pleasure to write a few welcome notes. With repect to catalysis, we live in exiting times. This holds both for developments in and the pace of scientific progress in understanding and designing catalysts , as well as for identifying new applications areas including scale-up to real world impact.

To mention just a few elements :

Recent advances in spectroscopic characterisation of catalyst particles and ensembles, including e.g. operando spectrocopy, enable whole new catalysis hypotheses. Multi scale catalysis charactererisation and design is a fast moving area.

Applications of catalysis in e.g. conversion of sunlight or catalytic conversion of biomass develop faster then ever and will have significant societal impact.

Unlocking the potential of these new and radically modified catalysts requires intimate interaction with process technology and engineering proncipiples.

More then ever, the world needs effective catalysis to contribute to some of the grand societal challenges ahead of all of us.

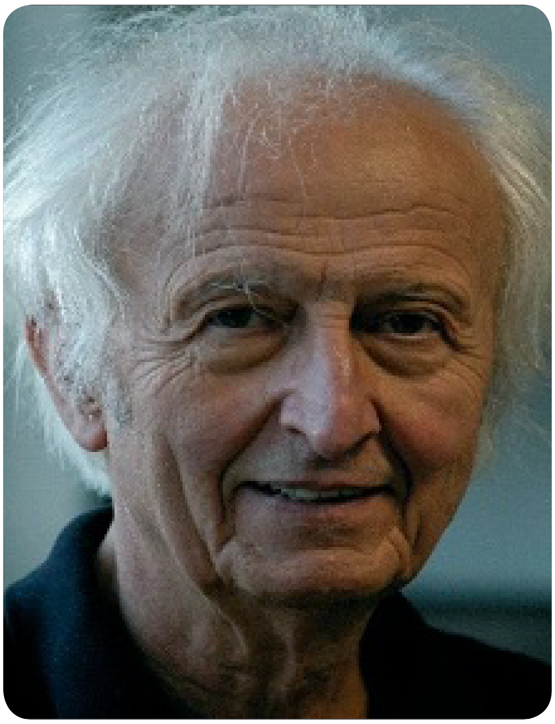
Q. B. Broxterman
InnoSyn B V
The Netherlands

Welcome Message

Dear participants, I would like to welcome you and write a few introductory notes. Catalysis is everywhere ! I am sure you would agree with me that the general theme of catalysis spans from biocatalysis, first mimicking Nature, via transition metal catalysis, electrocatalysis, organocatalysis, and many other subdisciplines, towards more traditional industrial heterogeneous catalysis using active sites on supports of various kinds. It is particularly the application of catalysis in industry that allows chemists and chemical engineers to make processes more cost effective by lowering energy consumption and more environment friendly by increasing the atom economy. As you know catalysis is one of the main principles of Green Chemistry and I believe that its role in modern science is still going to grow. That is why we all convened here to exchange experience and ideas and to interact not only on strictly professional but also on social basis.

Jan Cermak
J. E. Purkinje University
Czech Republic

Welcome Message



Dear Participants of CAT 2018:

It gives great pleasure to have been invited to writing down a few words of welcome. Catalysis occupies a central place in numerous manufacturing processes, and without catalysis society would lack access to food and medicine; actually, most of the daily things we take for granted require catalysis at some stage of making them. According to estimates of the world bank, roughly 20 % of the entire world economy is related in some way or another to chemical catalysis, an initially purely academic question on how to assist in making or breaking bonds in molecules by a "mediator", a catalyst. As you may know, in China the technical term "catalyst" means "matchmaker" – how appropriate!

This conference in Rome, I trust, will not only provide insight in latest findings in catalysis research, but will also act as a "matchmaker".

Helmut Schwarz

Helmut Schwarz
Technische Universität Berlin
Germany

Welcome Message

Dear congress visitors,

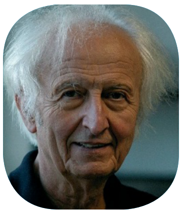
It is my honor and great pleasure to write a few welcome notes to you. Through centuries people were fascinated with the possibilities of synthesis of new materials with extraordinary properties. New materials are practically needed in all domains of life. Design and synthesis of new materials is one of the most important and interesting part of material sciences. Particularly a synthesis of new active and selective catalysts is a very important challenge. Our main aim concentrates on the new methods of the synthesis of single-site hierarchical porous zeolite catalysts with acid-base and redox properties. Such zeolite catalysts with active sites formed by incorporation of heteroelements in their framework are perspective as catalysts of protection of environment and biofeedstock conversion into valuable chemicals.

Stanislaw Dzwigaj

Stanislaw Dzwigaj
Sorbonne Universités
France

Keynote Speakers

Stanislaw Dzwigaj
Sorbonne Universités
France



Helmut Schwarz
Technische Universität Berlin
Germany

Christophe LEN
Chimie ParisTech
France

Bruno Zelić
University of Zagreb
Croatia

Jan Cermak
J. E. Purkinje University
Czech Republic

Q. B. Broxterman
InnoSyn B V
The Netherlands

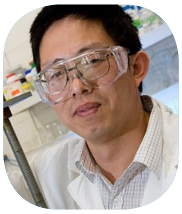
Christo Boyanov Boyadjiev
Bulgarian
Academy of Sciences, Bulgaria

Serge Cosnier
Grenoble Alpes University
France

Keynote Speakers

Luis Sánchez Granados
Universidad de Córdoba
Spain

Bruno Azambre
University of Lorraine
France



Zhonghua (John) Zhu
The University of Queensland
Australia

Pascal Granger
University of Lille
France

Luisa María Gómez Sainero
Universidad Autónoma
de Madrid, Spain

Valérie Meille
University of Lyon
France

Byeong-Kyu Lee
University of Ulsan
Republic of Korea

Juha Lehtonen
VTT Technical Research
Centre of Finland Ltd, Finland

About
MAGNUS GROUP

Magnus Group (MG) is initiated to meet a need and to pursue collective goals of the scientific community specifically focusing in the field of Sciences, Engineering and technology to endorse exchanging of the ideas & knowledge which facilitate the collaboration between the scientists, academicians and researchers of same field or interdisciplinary research. Magnus group is proficient in organizing conferences, meetings, seminars and workshops with the ingenious and peerless speakers throughout the world providing you and your organization with broad range of networking opportunities to globalize your research and create your own identity. Our conference and workshops can be well titled as 'ocean of knowledge' where you can sail your boat and pick the pearls, leading the way for innovative research and strategies empowering the strength by overwhelming the complications associated with in the respective fields.

Participation from 80 different countries and 688 different Universities have contributed to the success of our conferences. Our first International Conference was organized on Oncology and Radiology (ICOR) in Dubai, UAE. Our conferences usually run for 2-3 days completely covering Keynote & Oral sessions along with workshops and poster presentations. Our organization runs promptly with dedicated and proficient employees' managing different conferences throughout the world, without compromising service and quality.

About CAT 2018

On behalf of our organizing committee, we take an enormous pleasure in inviting you to attend the 2nd Global Conference on Catalysis, Chemical Engineering & Technology (CAT 2018) in September 13-15, 2018 at Rome, Italy.

The Conference is designed to facilitate the sharing of knowledge and experience of researchers, young inspired scientists, academicians, and industrialists worldwide. CAT 2018 will continue this philosophy by encouraging the sharing of research and practice of Catalysis and Chemical Engineering education, as it impacts on the learning experience of students and qualified practitioners and social care needs, and safety, of the individuals and communities it serves worldwide.

The theme of the conference is "Accentuate Innovations and Emerging Novel Research in catalysis and Chemical Engineering", will provide a forum for academia and industry to disseminate their latest innovations and practices. The focus is on present state-of-the art new ideas, practical considerations and novel applications in Catalysis and Chemical Engineering.

About Exhibitor

micromeritics®

The Science and Technology of Small Particles™

Micromeritics Instruments Corporation, a privately held company headquartered in Norcross, Georgia USA, is a leading global provider of high quality scientific instrumentation for material characterization. In business for over 55 years, Micromeritics offerings include techniques for characterization of density/volume, surface area and porosity, physical and chemical adsorption, size and shape of particles, porous materials and powders. In addition to designing, building and selling its own instrumentation, Micromeritics, under its Particulate Systems brand, also offers complementary OEM and private label instruments through the Micromeritics global sales channel and distributor partners. Micromeritics also operates fee-for-service testing, certification and methods development laboratories under the Particle Testing Authority and Porotechnology brands in Asia (Shanghai, China); the Americas (Norcross, GA / Kingwood, TX USA); and Europe (Aachen, Germany). Micromeritics also recently completed the acquisition of Freeman Technology Corporation, Ltd of Gloucestershire, UK adding significant capabilities and products for powder handling and characterization.

Micromeritics has also completed recently the acquisition of Process Integral Development S.L. (PID Eng &Tech). Its staff is formed by experts with multidisciplinary backgrounds in chemical engineering, electronics, automation and software engineering. PID Eng & Tech provides modular laboratory microreactor systems for the measurement of catalytic activity and for the study of yield and kinetics of chemical reactions. In addition, they offer standard pilot plant systems and specialized lab equipment. They also work closely with clients to design, build and commission bespoke pilot scale equipment. The target markets for PID Eng & Tech products and services include universities, research centers, and private sector industrial companies, whose activities are focused in the fields of basic chemistry, petrochemistry, environment, catalysis, agro-chemistry and food technology, supercritical fluid extraction and new energies.

About Exhibitor

BioLogic
Science Instruments

Bio-Logic Science Instruments SAS is a French designer and manufacturer of high performance laboratory research instruments and software. The headquarters are based in Seyssinet-Pariset, France (close to Grenoble in the French Alps).

Founded in 1983 by a CNRS researcher Yves Dupont and an industrial partner, Bio-Logic SAS is currently headed by François GOY.

Bio-Logic is a rapidly growing global company with affiliate offices as Bio-Logic USA, Bio-Logic India, Bio-Logic Middle East and Bio-Logic Spain, and has a large and growing network of worldwide distributors (with representatives in most large and developing countries).

Bio-Logic SAS has designed instruments for a variety of domains and applications:

- Electrochemistry
- Rapid-Kinetics, Spectroscopy & Photosynthesis
- Battery & energy devices testing
- Materials testing
- Electrochemical Scanning systems
- Electrophysiology

In 2012 Bio-Logic acquired Uniscan Ltd., a British specialist manufacturer of electrochemistry scanning instruments, expanding its product range in order to satisfy the expanding market of scanning electrochemical applications.

Bio-Logic’s team is continuously innovating and developing pioneer solutions to enable our customers in their research.

Publishing Partner

catalysts
an Open Access Journal by MDPI

Catalysts (ISSN 2073-4344; Impact Factor: 3.082) is an open access journal of catalysts and catalyzed reactions published monthly online by MDPI, providing a rigorous and rapid peer-review. Manuscripts are peer-reviewed and a first decision provided to authors approximately 14 days after submission; acceptance to publication is undertaken in 6.9 days (median values for papers published in this journal in 2017).

/Catalysts/ has been indexed by the Science Citation Index Expanded (Web of Science), Scopus and other databases (http://www.mdpi.com/journal/catalysts/indexing) and has 70,000-100,000 page visitors each month. According to web of science's data, the impact factor for /Catalysts/ 2016 is 3.082. The 5-year impact factor has risen to 3.947. Catalysts now ranks in Q2 of the "Chemical, Physical" category. According to Scopus data, CiteScore for /Catalysts/ 2016 is 3.44, which ranks in Q1 of the "Chemistry, Physical and Theoretical Chemistry" category, and Q2 of the "Chemical Engineering, Catalysis" category.

Note: CAT 2018 participants will receive a benefit of 25% waiver on article processing charges.

TABLE OF CONTENTS

DAY 1

KEYNOTE FORUM

2nd Global Conference on

Catalysis, Chemical Engineering & Technology

SEPTEMBER 13-15, 2018
ROME, ITALY

CONTENTS

Functionalization of porous materials for application in environmental catalysis for protection of environment

Stanislaw Dzwigaj, Ph.D.
Sorbonne Universités, UPMC, CNRS, France

Biography

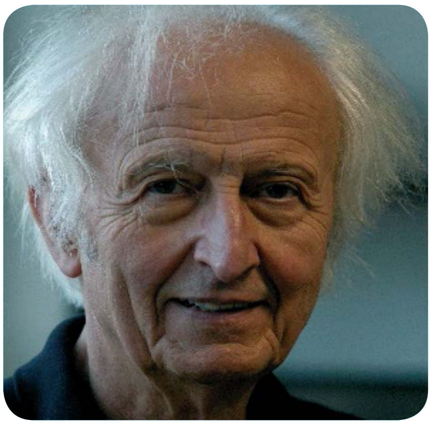
Professor Stanislaw Dzwigaj was trained in chemistry in Institute of Catalysis and Surface Chemistry, Krakow (Poland) where he obtained his PhD in Science in 1982 in the group of Prof. Jerzy Haber. After a postdoctoral stay at the Laboratoire de Réactivité de Surface Université P. et M. Curie (Paris, France) in the group of Dr Denis Barthomeuf (1987-1988) he obtained in 1990 a position of contract researcher in the same Laboratory devoted to surface reactivity in relation to catalysis phenomena. Then, in 2008 he obtained permanent position in CNRS as a researcher. On February 19, 2014 for outstanding scientific achievements he received the title of professor.

During my plenary lecture a functionalization of porous materials with transition metals such as Co, Fe, Ni and Cu will be discussed and obtained materials will be characterized with different physical techniques at the molecular and macroscopic levels. The porous materials with transition metals incorporated in their structure are applied in the different catalytic processes important for protection of environment such as selective catalytic reduction of NO_x to N_2 and hydrodechlorination of chlorinated volatile organic compounds into non-toxic, environmentally friendly products.

Audience Take Away:

- The audience will be able to understand as control of preparation of catalyst systems.
- They will see that catalytic activity depend on dispersion of metal in the framework of zeolite.
- The researchers will be able, after my talk, do their own catalyst preparation using similar method.

CONTENTS



Biography

Helmut Schwarz read chemistry at the Technische Universität Berlin (TUB) where, in 1972, he received his PhD and completed his habilitation in 1974. After having spent some time at the ETH Zürich, MIT, and Cam- bridge University, in 1978 he accepted a faculty position at TUB. Helmut Schwarz has occupied numerous visiting professorships on all continents, he has authored >1000 peer-reviewed articles and delivered an even larger number of (invited and named) lectures all over the globe. For his work on gas-phase chemistry and physics, Schwarz has received more than 50 distinctions and honors. After having served as Vice President of the German Research Foundation from 2001–2008, in January 2008 Dr. Schwarz was elected President of the Alexander von Humboldt Foundation.

Ménage-à-Trois: Single-atom catalysis, Mass Spectrometry and Computational chemistry

Helmut Schwarz, Ph.D.

Institut für Chemie, Technische Universität Berlin, Germany

We shall present selected examples of gas-phase reactions which are of timely interest for the catalytic activation of small molecules. Due to the very nature of the experiments, detailed insight in the active site of catalysts is provided and – in combination with spectroscopic studies and computational chemistry – mechanistic aspects of as well as the elementary steps involved in the making and breaking of chemical bonds are revealed.

Examples to be discussed include inter alia: (i) Metal-mediated carbon-carbon bond formation; (ii) low- temperature, catalytic oxidation of CO; or (iii) the coupling of NH_3 and CH_4 to produce HCN. Of particular importance are the reactions of "bare" metal-carbene complexes, when generated in the gas phase and exposed to thermal reactions under (near) single-collision conditions. In addition to the well-known metathesis and cyclopropanation processes, they exhibit rather unique reactivities. For example, at room temperature the unligated $[AuCH_2]^+$ complex brings about efficient C□C coupling with methane to produce C_2H_x ($x = 4, 6$), or the couple $[TaCH_2]^+/CO_2$ gives rise to the generation of the acetic acid equivalent $CH_2{=}C{=}O$. Entirely unprecedented is the thermal carbon-atom extrusion from halobenzenes (X = F, Cl, Br, I) by $[MCH_2]+$ (M = La, Hf, Ta, W, Re, and Os) and its coupling with the methylene ligand to deliver C_2H_2 and $[M(X)(C_5H_5)]^+$. Among the many noteworthy C□N bond forming processes, the formation of CH_3NH_2 from $[RhCH_2]^+/NH_3$, the generation of $CH_2{=}NH\ ^+$ from $[MCH2]^+/NH_3$ (M = Pt, Au), or the production of $[PtCH{=}NH_2]^+$ from $[PtCH_2]+/NH_3$ are of particular interest. The latter species are likely to be involved as intermediates in the platinum-mediated, large-scale production of HCN from CH_4/NH_3 (DEGUSSA process). In this context, a few examples are presented that point to the operation of co-operative effects even at a molecular level. For instance, in the coupling of CH_4 with NH_3 by the heteronuclear clusters $[MPt]+$ (M = coinage metal), platinum is crucial for the activation of methane, while the coinage metal M keeps control on the branching ratio between the C□N bond forming step and unwanted soot formation.

It will be shown that mass-spectrometry based studies on 'isolated' reactive species provide an ideal arena for probing experimentally the energetics and kinetics of a chemical reaction in an unperturbed environment at a strictly molecular level, and thus enable the characterization of crucial intermediates that have previously not been within the reach of conventional condensed-phase techniques. Clearly, these investigations open the door to a widely uncharted territory of chemistry, a field in which "each atom counts".

Biography

Prof. Dr Christophe Len is a Full Professor at the Université de Technologie de Compiègne – UTC (France) and performs his research in PSL Research University, Chimie ParisTech. He has published almost 160 original publications and review articles, 7 chapters and 8 patents (H-index 24). Among recent awards and recognition to his scientific career, he was promoted Honorary Professor of the University of Hull, England (2012-2018), Honorary Life Fellow of Indian Society of Chemists and Biologists (ISCB, 2014), Fellow of the Association of Carbohydrate Chemists and Technologist of India (ACCTI, 2015) and Fellow of the Royal Society of Chemistry (FRSC, 2015). Moreover, he received Glycerine Innovation Research Award (2017). His current research explores organic chemistry and catalysis applied to biomass using alternative techniques.

Catalysis in/on water: Future perspectives

Christophe LEN, Ph.D.
Chimie ParisTech, France

The design of environmentally friendly methodologies has been the driving force of scientists in recent years. In particular, the use of biomass-derived materials, green solvents and alternatives techniques has been investigated.

In this presentation, several green chemistry approaches that target advanced synthesis and processes will be presented. These approaches include: (i) C-C bond formation such as Suzuki-Miyaura, Heck and Tsuji-Trost cross coupling reactions in water; (ii) homogeneous and heterogeneous catalysis as well as micellar catalysis in water; (iii) alternative technologies such as microwave irradiation, high temperature/pressure, ultrasound irradiation; (iv) continuous flow processes assisted by microwave irradiation, ultrasound irradiation or not.

Conception, synthesis and physico-chemical properties will be detailed.

Audience Take Away:

- Use of alternative technologies in place of traditional processes
- Use of clean solvents instead of toxic solvents
- Use of biomass feedstocks instead of fossil resources

Biography

Bruno Zelić received his PhD in chemical engineering in 2003 at University of Zagreb. From 2012 he is full professor at the Faculty of Chemical Engineering and Technology, University of Zagreb. His research interests are in the field of implementation of microreactor technology into biotechnology. More than 80 scientific and professional publications, 2 patents, and more than 60 oral (plenary, key note, invited) and poster presentations on the international conferences present his scientific work. Bruno Zelić was dean of the Faculty of Chemical Engineering and Technology, University of Zagreb from 2013 to 2017. Currently, he is a member of Executive Board of European Federation of Chemical Engineering and Editor-in-Chief of Chemical and Biochemical Engineering Quarterly journal.

Fully integrated biotransformations in a microreactor

Bruno Zelić, Ph.D.
University of Zagreb, Croatia

Nowadays, microreactors are finding more and more applications in different fields of chemical and pharmaceutical industry, biotechnology and medicine. The application of different microreactor systems in intensification of the biochemical production processes is widely studied. Some researches claim that 50 % of reactions in the fine chemical or pharmaceutical industry could benefit from a continuous process based mainly on microreactor technology, and for the majority (44 %) a microreactor would be the preferred reaction device.

Decreased channel dimensions of microreactors (on the order of 10 – 500 µm) afford numerous advantages that lead to increased reaction efficiency. A high surface to volume ratio, faster diffusion dominated transport, enhanced heat transfer and thus reduced energy demands, good process control, high throughput, usage of minimal (microliters) of reagent volumes, etc., are some of a microreactor advantages that are usually stressed. Microreactors could be easily coupled with numerous detection techniques together with the pretreatment of the samples on the one single unit. Having in mind all those benefits one of the main motivations for the use of microreactor technology is the gain in the yield and safety.

Although a great majority of the reaction systems that are studied in microreactors are connected with chemical synthesis, biocatalysis and biotransformations in a microreactor are demonstrated as promising alternative. Syntheses, oxidations, transesterifications, polymerizations, hydrolyses and coenzyme regenerations catalysed by enzymes or whole cells are just some of numerous different biotransformations that have been successfully performed in microreactors.

Microreactor advantages in biotransformations will be demonstrated on three case studies, namely, (i) alcohol dehydrogenase catalyzed hexanal production with in situ NAD^+ cofactor regeneration and product separation, (ii) two-phase aqueous extraction of polyphenols and, (iii) biocatalytic production of biodiesel using an enzyme lipase with integrated biodiesel purification.

Audience Take Away:

- Application of microreactors in biocatalysis and biotransformations
- in situ cofactor regeneration in a microreactor
- in situ purification of products in a microreactor
- Use of enzyme immobilized on magnetic nanoparticles in a microreactor

CONTENTS

Biography

Jan Čermák received his PhD in 1986. He was a postdoc with Professor Bernard L. Shaw (University of Leeds, UK, 1992-93), and Visiting Scientist with Professor Walter Leitner (MPI Mülheim, Germany, 2001). He became Associate Professor of Organic Chemistry in 2008. Currently, besides continuing his work at the Czech Academy of Sciences (as Senior Research Scientist, previously Head of Department and Institute's Deputy Director), he is Head of Department of Chemistry at J.E. Purkinje University, Ústí nad Labem, Czech Republic. His research interests include organometallic chemistry of transition metals and catalysis in one- and biphase systems. He serves as Chair of the Division of Organometallic Chemistry of EuCheMS (2014-2020).

Fluorous ponytails in catalysis

Jan Čermák, Ph.D.

Institute of Chemical Process Fundamentals of the CAS, v.v.i., Czech Republic
J. E. Purkinje University, Czech Republic

Fluorous chemistry started in 1994 after publication of the seminal paper by József Rábai and István Horváth in Science. Despite being introduced as a tool for catalysis, it later developed also into powerful instrument of organic chemistry. To return back to its originally intended use in catalysis, careful design (tailoring) of catalysts was needed, be it transition metal complexes with fluorous ponytails or fluorous ponytailed organocatalysts. Principles of the design of fluorophilized catalysts of both types will be presented together with the methods of characterization of both the molecular structure and fluorophilicity of the compounds. The examples will be taken from the work of our group and also from the work of others. In transition metal catalysis we were interested in fluorophilized cyclopentadienyl complexes with metals like titanium, rhodium and iridium and recently also in NHC complexes of the late transition metals. Cyclopentadienyl complexes of several types were prepared and it was shown that the ease of synthesis and also their properties strongly depend on the way of attaching fluorous ponytails to the parent structure. Dynamic behavior of the complexes was often observed showing promise concerning their use in catalysis.

Our recent synthesis of a new type of fluorous tag led us into the underdeveloped area of fluorous organocatalysts since for some purposes relatively expensive transition metals should be avoided. Further expansion of the methodology in terms of solvent use will be also presented. It is known that fluorous componds are well compatible with such environment-friendly solvent like supercritical carbon dioxide. In addition to examples from the work of others, our results of catalysis in supecritical carbon dioxide will be shown.

Audience Take Away:

- The understanding of the concepts of fluorophilicity and fluorous biphase systems and their variants will be embraced.
- Principles of synthetic design of compound fluorophilized by fluorous ponytails will be communicated.
- The presentation of numerous examples of synthesis and catalytic use of fluorous materials both in fluorous systems and in supercritical carbon dioxide should help the audience in solving their own experimental problems concerning the catalyst separation and recycling.

DAY 1

SPEAKERS

2nd Global Conference on

Catalysis, Chemical Engineering & Technology

SEPTEMBER 13-15, 2018
ROME, ITALY

Effect of temperature on Cr promotion of Mo_2C supported on sulfated Zirconia for methane dehydroaromatization

James J. Spivey*, Ashraf Abedin, Swarom Kanitkar, Srikar Bhattar
Cain Department of Chemical Engineering, Louisiana State University, USA

The shale gas revolution has made immense and previously unattainable resources of natural gas accessible and economically competitive. A major component of natural gas is methane, which is typically used for power generation or is flared. Methane dehydroaromatization (MDHA) is a process in which methane can be converted into valuable hydrocarbons, including ethylene and benzene. Mo oxide supported on ZSM-5/MCM-22 has been well-studied in recent years for MDHA. It is generally thought that Mo carbides are responsible for activating methane by forming CH_x species. These are dimerized into C_2H_y species, which are then oligomerized on the acidic zeolite sites available on ZSM-5/MCM-22 support, leading to aromatics. In these catalysts, sulfated zirconia (SZ) can provide the acid sites. In present work, Cr is introduced as promoter for Mo_2C/SZ. Cr has been previously added along with other metals in ZSM-5 in the form of extra-framework species to facilitate the catalyst dehydrogenation function for MDHA. 0.5 wt. % of Cr was added to a 5 wt.% Mo/SZ by incipient wetness impregnation. DRIFTS was use to characterize the surface acidity of chemisorbed pyridine.

The reactions were run at 600ºC, 650ºC and 700ºC for 15 hours to study the promotional effect of Cr for MDHA. The catalyst was first reduced under H_2 till it reached the desired reaction temperature. It was carburized subsequently under 1:4 CH_4:H_2 ratio for 4 hours before starting the reaction. Products observed were ethylene, ethane, propylene, with aromatics including benzene, toluene and ethylbenzene. The promotion of Cr increased with temperature, as observed by higher methane conversion as well as high ethylene and benzene yield. However, at higher temperatures, deactivation occurred rapidly. This was likely due to coking on catalytic surface, later confirmed by TPO.

Audience Take Away:

- A new catalytic approach for MDHA, Bifunctional catalytic system, Promotional effect of Cr for higher Benzene yield in MDHA
- The audience will be introduced to a new promoter (Cr) for Mo_2C/SZ catalyst for MDHA which shows higher methane conversion and benzene yield than the Mo_2C/SZ catalyst without Cr. A comparison of current Mo-ZSM-5 catalysts reported in the literature showed higher activity for the Cr-promoted Mo_2C/SZ catalyst. This will suggest other alternate catalysts for MDHA.
- The audience will learn a newly proposed mechanism of MDHA catalytic reaction. The catalysis community will learn about the acidic effect of the Cr-promoted Mo_2C/SZ that replaces the conventional HZSM-5 as well as the promotional role of Cr in Mo_2C/SZ catalytic system. This will describe new alternatives to MDHA processes.

Biography

James Spivey is Eidt and McClaren Professor of Chemical Engineering at Louisiana State University. His research focuses on catalytic conversion of methane and hydrocarbons, and characterization of related heterogeneous catalysts. He is Editor-in-Chief of Catalysis Today (Elsevier) and Catalysis SPR book series (Royal Society of Chemistry).

CONTENTS

Stabilization of hydrolytic enzyme(s) for commercial application

Simone De Rose[1], Halina Novak[1], Andrew Dowd[2], Sukriti Singh[2], Jennifer Littlechild[1], Dietmar Andreas Lang[2*]
[1]Henry Wellcome Building for Biocatalysis, Biosciences, College of Life and Environmental Sciences, University of Exeter, Stocker Road, Exeter EX4 4QD, UK
[2]Unilever R&D, HomeCare Discover, Disruptive Biotechnology, Quarry Road East, Bebington CH63 3JW, UK

In 2001 Sheldon and co-workers patented the method for the production of Cross-Linked Enzyme aggregates. The preparation of CLEAs involved the precipitation of the enzyme followed by crosslinking of the precipitated enzyme aggregates with a bifunctional crosslinking agent such as glutaraldehyde. The cross-linking occurs between amino groups of the lysine residues on the surface of the enzyme and the aldehyde group, the formation of covalent bonds, makes the CLEAs permanently insoluble. This method is robust and straightforward, and the CLEAs are significantly more stable to denaturation by proteolysis, heat and organic solvents than the corresponding soluble enzyme.

A commercial variant of Thermomyces lanouginosa lipase (Lipex 16L) has been used to develop an improved method for CLEAs production, with applications in detergent products. Lipex 16L differs from the wild-type T. lanouginosa lipase due to two mutations (T231R, N233R) which improve wash performance and show beneficial synergistic results when combined with bleach catalysts. Lipex 16L is widely used in the laundry industry where it is considered one of the benchmark enzymes.

A new improved immobilization method has been developed and compared to a commercially available CLEA. It has been shown to be able to prepare homogenuous particles which are more active than the free enzyme and that these immobilised enzymes are suitable for HPC applications.

Audience Take Away:

- The technology can be applied to stabilize enzymes to be used in other processes, such as biocatalysis.
- Combing chemicals with biomolecules to produce "rigid" bio-conjugates molecule with improved properties, excellent for research and teaching purposes.
- Defined CLEAs, especially particle size, are more accurate and provide more performance than larger particles.

Biography

Dietmar Lang completed BSc/MSc in Biotechnology, and a Ph.D. in Structural Biology / Protein X-ray crystallography, both from the University of Technology, Braunschweig (1995, Germany) and a Master in Pharmaceutical Medicine from University of Witten-Herdecke (1999, Germany) followed by Post-Doc years in Groningen (NL) and European Molecular Biology Laboratory (D). In 1999 joined health care provider Fresenius Medical Care (D), managing medical research in renal replacement therapy. In 2002, move to Swiss company (Siegfried), developing biosimilar biopharmaceuticals – product by bioprocess. Changing to Lonza Biologics (2008, UK) did allow to do some cutting-edge innovative bioprocess related development projects for novel biopharmaceuticals. As Associate Director Program Management for companion diagnostics development at Qiagen (2010, UK) he led cross-functional project teams for the development of FDA approved diagnostic technology in conjunction with Active Pharmaceutical Ingredients. Five years ago (Unilever, 2013), he went back into the field of industrial enzyme research where his scientific career started, leading the biotechnology platform for Home & Personal Care at Unilever.

In situ studies of model catalysts for heterogeneous catalysis

Hans O. A. Fredriksson[1]*, J. W. Niemantsverdriet[2], Yibin Bu[3]
[1]Senior research scientist, Syngaschem BV, Netherlands
[2]Director, Syngaschem BV, Netherlands
[3]Associate researcher, Southern University of Technology and Science, China

Catalysis research is complex and multidisciplinary in its nature. The performance of an industrially used catalyst is determined by a multitude of factors, from material composition to oxidation state, support porosity, reactant and product distribution in the reactor as well as temperature gradients and local hot spots. Therefore, under "real" conditions, it is nearly impossible to learn which are the most important properties of a catalyst. By preparing simplified model systems, it is possible to eliminate some of the variables during catalyst testing and learn about the materials fundamental properties. We prepare flat model catalysts, consisting of merely a few μg of catalytically active material and test them in a custom made micro reactor with in-situ mass spectrometry and UV-vis spectroscopy. The flat model catalysts have the advantage that there are no hot spots or diffusion limitations in the gas phase that can obscure the findings and that all catalyst material is accessible to in-situ characterization. A few examples will be presented, where we the importance of the oxidation state of the active material and the interaction between catalyst, support and promoter is elucidated.

Audience Take Away:

- The audience will learn how a micro reactor can be designed that allows them to test the catalytic properties of precisely designed model catalysts, with extremely low loadings of active material. This is valuable if the catalyst preparation technique is demanding, as for example with lithographically prepared samples or for catalysts where mass selected nanoclusters are used. They will also learn how this microreactor has been used to reveal the importance of catalyst oxidation state, which sometimes is different for the bulk and for the surface. Furthermore, the importance of in-situ catalyst characterization will be made clear.

Biography

Hans Fredriksson obtained his MSc degree in Physics at Gothenburg University in Sweden. In 2009, he completed a PhD in material science at the department of applied physics at Chalmers University of Technology in Gothenburg in the field of nanofabrication. In particular, he worked on model systems for catalysis and nano-optics research. In 2010, Hans joined Prof. Hans Niemantsverdriet's group at Eindhoven University of Technology to further pursue his interest in combining nanofabrication and catalysis research. His research topics ranged from the properties of catalysts for purification of the products of biomass gasification, and for methanol production from syngas to various micro reactor concepts and the work included daily supervision of PhD students. In January 2016, Hans joined Syngaschem BV. His focus is on investigating fundamental properties of catalysts and correlating these with activity and deactivation using model catalysts, micro reactors and a broad range of characterization techniques. He has (co-) authored around 20 research papers on various topics.

CONTENTS

Electrocatalytic conversion of organic compounds at solid/liquid interface from *Ab Initio* molecular dynamics simulations

Mal-Soon Lee[1]*, Sneha A. Akhade[2], Vanda Glezakou[1], Roger Rousseau[1]
[1]Senior Scientist, Institute of Integrated Catalysis, Pacific Northwest National Laboratory, Washington, USA
[2]Research Associate, Institute of Integrated Catalysis, Pacific Northwest National Laboratory, Washington, USA

Electrocatalytic conversion of biomass derived feedstocks offers a promising avenue for effective carbon recycling from renewable energy resources. To retain economic viability of this target technology, rational design of electrocatalysts with high activity and selectivity towards producing value-added chemicals and fuels is necessary. For improved conversion of biomass resources to fuels and fine chemicals, understanding and controlling the aqueous-phase catalytic hydrogenation of organic compounds on metals is crucial. Unlike gas-phase hydrogenation, the presence of water and the solid/liquid interface play critical roles in catalysis. Although there have been extensive studies in electrocatalysis, there exists a lack of mechanistic exploration and molecular-level understanding of electrocatalytic conversion of organic compounds specifically pertaining to biomass feedstocks. Moreover, these reactions occur at the solvated electrode-electrolyte interface where complex interactions between the electrode and solvent molecules have a critical influence on the reaction chemistry. In this talk, we will address the effect of the solvent and the charged metal electrode on the reaction pathways and their capacity to undergo reduction/hydrogenation. Results of molecular-scale structural/electronic properties near the electrochemical interface and the reaction energetics of target organic compounds obtained from density-functional-theory (DFT) based ab initio molecular dynamics (AIMD) simulations will be presented. The inferences drawn will be used to postulate design criteria for electrocatalytic conversion of organic compounds from an experimental and theoretical perspective.

Audience Take Away:

- The role of solvent in reaction mechanism
- This study will provide design criteria to improve electrochemical conversion of organic compounds on metal surface

Biography

Mal-Soon Lee is a senior scientist at Pacific Northwest National Laboratory. She has been working in the field of computational physics and chemistry with an emphasis on studying the phase behavior and reactivity at complex interfaces using a variety of statistical mechanical tools. Her areas of application include studies of catalysis, CO_2 sequestration, nuclear waste disposal, and high-pressure physics. To understand the entropy and enthalpy components of reactivity of these heterophase materials, large-scale high-performance computing techniques, such as ab initio molecular dynamics and/or ab initio electronic structure calculations, are employed. With these simulations statistical mechanical techniques are applied to calculate various properties such as enthalpies/entropies of reaction, spectroscopic properties, which can be directly compared with experimental observations.

Overview of radioactive cesium removal from nuclear wastes

Changhyun Roh, Ph.D.
Korea Atomic Energy Research Institute (KAERI), Republic of Korea

After the Fukushima Daiichi Nuclear Power Plant disaster in Japan in 2011, the demand drastically increased for efficient technology for the removal of radioactive cesium. Many researchers have suggested using physical adsorption methods to remove radioactive cesium from contaminated water. For example, polymers, nanocomposites, and clay have all previously been investigated for their capacity to remove radioactive cesium through the interaction between the negatively charged surfaces of naturally occurring adsorbents and the positive charge of radioactive cesium. However, powder-type adsorbents cannot be used to treat contaminated water in a real, open environment because there is no easy way to collect the adsorbents after they are used. In particular, adsorbents can cause blocking phenomena, which could be addressed by encapsulating the adsorbents with suitable modification that could alleviate the clogging and resolve the post-treatment separation problem. Therefore, novel solid absorbents are needed to allow easy separation of the materials from the contaminant environment to prevent secondary contamination. In this talk, I will overview the adsorbents for the efficient removal of cesium from nuclear wastes.

Audience Take Away:

- Synthesis of environmental catalyst for removal of radioactive cesium and recent overview nuclear wastes
- Understanding of nuclear energy and decontamination research

Biography

Changhyun Roh received his Ph.D degree at the Department of Chemical and Biological Engineering, Seoul National University, Seoul, Republic of Korea in 2007. Now he is Senior Researcher/Associate Professor at Korea Atomic Energy Research Institute/University of Science and Technology, Republic of Korea. His current research interests include functional materials, environmental science, nanotechnology, biotechnology and interdisciplinary research. He has published more than 70 research articles in SCI(E) journals. Several projects are ongoing as a project investigator.

CONTENTS

Hybrid catalysis: A new one-pot reactor for the valorisation of glycerol through heterogeneous and enzymatic catalysis

Myriam Frey*, Ph.D., D. Richard, Ph.D., P. Fongarland
LGPC (Lyon), France

The study we will present is part of the GLYCYBRIDE project whose aim is to develop a synergy between enzymatic and heterogeneous catalysis in a one-pot reactor to transform glycerol into value-added chemicals.

Our aim is to design a one-pot reactor able to perform three phase hybrid catalysis, one step being oxidation. Knowing that enzyme and heterogeneous catalysis require different reaction conditions, such as temperature, stirring speed, oxygen concentration (oxygen possibly inhibiting the enzymatic reaction), we designed a new reactor able to combine those two kind of catalysis. In order to validate the design of the reactor, we use a model reaction with two well-known steps (mechanism, kinetic parameters). One step requiring an efficient mass transfer of oxygen like the target reaction. Moreover, the media of both step should be compatible. The first reaction is an equilibrated enzyme catalyzed isomerization. The equilibrium of the first reaction will be shifted by a heterogeneously catalyzed oxidation.

In the present work, we performed a preliminary study to check the compatibility of reaction media. Then we studied separately the kinetics of both steps in order to provide a kinetic model of the reactions to simulate the designed reactor. First with a simple approach of a one-pot isothermal slurry reactor, which will be considered as a starting point for a more elaborated compartmentalized reactor model.

A first one-pot slurry simulation was run by using kinetic laws and data collected from the literature. This model requires adjustments to describe the experimental data, especially for the oxidation reaction step, because the catalyst used was different from the one in the literature. For the enzymatic step, only minor adjustment should be necessary since the catalyst used is exactly the same as in the literature.

The compatibility of reaction media for both catalyst was checked. The enzyme requires stable pH conditions, low-moderate speed of agitation. Blank tests first confirmed that without catalyst no reaction occurred in the reaction conditions (temperature, buffer) that are to be used. The isomerization step kinetics is not impacted by the use of phosphate buffer or the presence of air necessary for the second step. In addition, low stirring speed (200-300 rpm) is sufficient to prevent diffusion limitations. For the oxidation step, the use of phosphate buffer has no significant effect on the reaction kinetics. For both steps, kinetic parameters had to be estimated in order to fit the simulation of the one-pot slurry model to the experimental data.

Finally, a first one-pot slurry test was performed and showed that both steps could indeed be combined. Fructose was converted into glucose, which was seen to be continuously oxidized into gluconic acid. However, the conversion was different from the expected one. Further investigation is under progress to understand why and to tune the experimental conditions and find an optimum for the coupling of both steps.

Audience Take Away:

- The lecture will bring knowledge about a new trend in the catalysis field: hybrid catalysis and the complexity of associating enzymatic and heterogeneous catalysis for a one-pot reaction
- A new design of reactor for one-pot hybrid catalysis, whose design will be validated by an appropriate model reaction that had to be developed
- The importance of model reaction as proof of concept, how to use this model reaction to validate the design of the reactor developed

Biography

After obtaining a Life Science bachelor's degree specialized in Chemistry and Biology (2010), followed by a Master's degree in Green Chemistry (2012) in Strasbourg University. For PhD degree in Chemical Engineering (2012-2016), I studied the optimization of an open cell foam platelet milli-reactor for the intensification of an exothermal reaction: the CO_2 methanation, at ICPCEES (Strasbourg). After that I spend one year at IC2MP (Poitiers) as post-doctoral researcher on an industrial project for Biosynthesis on the valorization of bio-sourced organic acids. I am now at LGPC (Lyon), as post-doctoral researcher, where I am working on the GLYCYBRIDE project, for which we are currently designing a one-pot reactor in order to transform glycerol into value-added chemical through a synergy between enzymatic and heterogeneous catalysis (hybrid catalysis).

CONTENTS

Quantum effects with fluid movement along the solid surface

Zamakhaev Victor, Ph.D.
Head of Science at Terratec LLC, Russian Federation

Worldwide in various industries and transport must deal with irregular effects associated with fluid flow along a solid surface. These effects are accompanied by not only the failure of the equipment, but often the people deaths and environmental disasters. The indicated effects cannot be explained based on classical physical representations. Disruption of fuel delivery in aviation and automobile engines during traffic (most often during forcing traffic); ejection from the well drilling string during deep hole drilling and problems with obtaining inflows from oil and gas reservoirs have the same physical basis. Chemisorbed gas molecules (carbon dioxide) are easily excitable in the infrared and acoustic ranges. This gas is widely distributed in nature and it is a part of natural gases. Because of carbon dioxide we often encounter quantum effects.

In a coherent system on the surface of a solid body, all pulses are radiated in a strictly defined direction. The momentum from the molecule to the molecule will grow rapidly enough. And at the end of the drilling column (at the wellhead) this momentum will generate pressure up to tens of thousands of MPa. In addition to impulse action, coherent reactions are possible.

We should not lose sight of the positive aspects. For instance, nowadays some technologies for increasing oil recovery and flow rates of wells at depleted oil fields are developing based on quantum effects.

Based on the huge experimental material, the author concluded that bodies or systems of particles with a catalytically active surface that are at least temporarily in a gas-liquid medium of a certain composition of gases can create in the subsurface layer of each solid body waves that ensure the mass transfer of this body in a conventional liquid with high velocities.

Audience Take Away:

- The developments described in the report will avoid many accidents and environmental disasters.
- To create new technologies for increasing oil recovery and to produce oil from low-permeability reservoirs.
- Create fundamentally new engines with extremely high efficiency.

Biography

Victor Zamakhaev earned his PhD degree in the field of physics of reservoir from Moscow Engineering and Physical Institute. For a long time, he worked for All-Russian Scientific Research Design Institute of Explosive Geophysics where he was head of well completion and testing department. Also, he has taken different position at Gubkin Russian State University of Oil and Gas during the past fifteen years. Victor Zamakhaev is the author of many books and articles at the field of petroleum engineering. His research work is directed to processes in petroleum reservoirs under filtration and dynamic stimulation.

Metal based electrocatalysts on CeO_2/carbon, Nb_2O_5/carbon and carbon: Synthesis, characterization and investigation of their electrocatalytic activities for both anodic and cathodic fuel cell reactions

Virginija Kepenienė*, Ph.D., Raminta Stagniūnaitė, Ph.D., Daina Upskuvienė, Ph.D., Vidas Pakštas, Ph.D., Algirdas Selskis, Ph.D., Loreta Tamašauskaitė-Tamšiūnaitė, Ph.D., Eugenijus Norkus, Ph.D.
Center for Physical Sciences and Technology, Lithuania

A fuel cell is electrochemical cell that converts chemical energy into electrical energy without intermediate of mechanical links. Fuel cells are different from batteries in requiring a continuous source of fuel and oxygen (usually from air) to sustain the chemical reaction, so it is very important to select suitable catalysts for both oxidation of the fuel and reduction of oxygen. Nanoscale materials are very important in many industries. There are many various synthesis methods such adsorption, electroless deposition, galvanic displacement or microwave irradiation methods which let to fabricate nanomaterials. Nanoparticles-based catalysts are usually heterogeneous catalysts broken up into metal nanoparticles in order to speed up the catalytic process. Metal nanoparticles have a higher surface area so there is increased catalytic activity because more catalytic reactions can occur at the same time. Nanoparticle catalysts can also be easily separated and recycled with more retention of catalytic activity than their bulk counterparts.

In the present work, Pt, Au and Co nanoparticles deposited on the different surfaces such as CeO_2/carbon, Nb_2O_5/carbon or carbon were fabricated using the rapid microwave heating and adsorption methods. The synthesized catalysts were examined by Transmission Electron Microscopy, X-ray Diffraction and Inductively Coupled Optical Emission Spectroscopy. The electrocatalytic activity of the Pt, Au and Co supported catalysts towards the oxidation of alcohols and reduction of oxygen was investigated by cyclic voltammetry, chrono-techniques and rotating disk electrode linear sweep voltammetry.

Metal nanoparticles of ca. 1-15 nm in size were successively deposited onto the surfaces of CeO_2/carbon, Nb_2O_5/carbon and carbon. Metal nanoparticles were uniform and well dispersed on the mentioned surfaces.

It has been found, that the modified catalysts show enhanced electrocatalytic activities towards alcohols oxidation as well as oxygen reduction reactions in comparison with those at the bulk platinum or gold catalysts.

Audience Take Away:

- The audience will learn basic knowledge about the fabrication and application of nanocatalyst for fuel cell.
- There will be discussed and compared nano-scale materials prepared by to different methods as microwave irradiation heating and adsorption.
- There will be discussed specific details on particular processes: fuel (methanol, ethanol, ethylene glycol) oxidation reaction; oxygen reduction reaction.

Biography

Virginija Kepenienė got her PhD degree in 2012 at the Department of Catalysis of Center for Physical Sciences and Technology (FTMC) on an electroless deposition in the group of Prof. Eugenijus Norkus. After a post-doctoral internship related to the investigation of catalysts for alkaline fuel cells at the FTMC in the group of Dr. Loreta Tamašauskaitė-Tamašiūnaitė (2013-2015) she continued her work as a researcher at the same Department in relation to synthesis and investigation of various nano-scale materials for fuel cell reactions. She has been working as a senior researcher since 2017. Virginija Kepenienė actively participates in scientific activity: carries out experimental investigations, participates in projects as well as in students training, supervises Bachelor's, Master's and PhD's works and students practice projects. She is co-author of 21 publications, among them 16 keynote author. 47 contributions to conferences, of which 25 is the keynote speaker. Co-author of the Lithuanian patent.

Laccase detoxification of lignocellulose biomass to improve their conversion to chemicals

Iris Cornet*, Valentin Sóti
Faculty of Applied engineering, Research Group Biochemical Green Engineering & Materials (BioGEM), Antwerp University, Salesianenlaan 90, 2660 Hoboken, Belgium

The conversion process of lignocellulose to chemicals, such as, ethanol, lactic acid or oleochemicals, consists of four main steps, i.e., pretreatment, hydrolysis, fermentation and downstream processing, often performed in simultaneous processes which decreases the process time and product inhibition.

In the present research, poplar wood was pretreated by steam explosion and two fractions were obtained, i.e., the solid glucose rich fraction and the liquid xylose rich fraction. Both fractions also contain phenolic degradation products of lignin which have an inhibitory effect on the hydrolyzing enzymes and the fermenting microorganisms. During the hydrolysis, the polysaccharides are cut to monosaccharides. Due to inhibition by lignin, the yield is lower and less sugar can be obtained from a certain amount of biomass. Therefore, it was first investigated how commercial laccase enzymes may positively affect the enzymatic hydrolysis reaction of polysaccharides to monosaccharides, by oxidizing the lignin-derived phenolics. After this, so-called, laccase detoxification, hydrolysis was performed and it was investigated whether it gave a better result. The experiments showed that the presence of solids significantly altered the reaction performance of the laccase enzyme and that, dependent on the applied enzyme, laccase reaction was improving hydrolysis or decreasing its efficiency.

As enzyme cost is considered to be one of the main factors that define the process costs, enzyme immobilization and recycling was researched. However, the solid particles present in a simultaneous saccharification and fermentation process (SSF) will prevent recovery of the enzymes by centrifugation or filtration. Moreover, solid particles are preferably in high concentrations which further increases the problem. Therefore, the use of magnetic immobilized enzymes (m-CLEAs) was investigated experimentally and from liquid medium, 99.5 m/m% of m-CLEAs could be recovered by a magnet in one step, while 88 m/m% could still be recovered from the high-solids SSF fermentation broth.

In the presentation, the reactor set-up in high-solids conditions, the enzyme recuperation and the enzyme costs will be discussed.

Audience Take Away:

- The audience will learn in what way the reaction environment of the laccase enzyme influences their behavior.
- The encountered problems and some practical solutions when using enzymes in high-solids reaction will be discussed.

Biography

Iris Cornet graduated as Bioengineer at the Vrije Universiteit Brussel (VUB). She started her career as a researcher on a collaborative project between VUB and Artois Brewery and continued to work at the VUB, in the Chemical engineering department. Afterwards, she was working at the Artesis University College. Additionally, she conducted research at the laboratory of Genetics and Microbiology, VUB. She finished a PhD at BioTeC, KULeuven, Belgium, on modelling of stress adaptation of E. coli. From 2014 on, she is employed at the Antwerp University. Her research focuses on using microorganisms and enzymes for valorisation of waste streams for industrial production of chemicals. Different fermentation strategies, such as solid state fermentation, high solids fermentations as well as submerged fermentations are applied. Her teaching assignment at the Faculty of Applied Engineering covers the fields of industrial biotechnology and bioprocess engineering.

CONTENTS

The Nanomaterials application for syngas processing

Kulikova Maya Valer'evna[1]*, Ph.D., Khadziev S. N[2], Ivantsov M.I[3], Chudakova M. V[4], Ph.D., Dement'eva O. S[5], Ph.D.
[1]Head scientist researcher, Chief of the Department, A.V.Topchiev Institute of Petrochemical Synthesis, Russian Federation
[2]D.Sc. in Chemistry, Professor, Academician of RAS, A.V.Topchiev Institute of Petrochemical Synthesis, Russian Federation
[3]Junior researcher, A.V.Topchiev Institute of Petrochemical Synthesis, Russian Federation
[4]Researcher, A.V.Topchiev Institute of Petrochemical Synthesis, Russian Federation
[5]Senior researcher, A.V.Topchiev Institute of Petrochemical Synthesis, Russian Federation

In recent years, nanoscale metal-contaning materials as catalysts for the syngas processing have increasingly garnered the interest of the researchers. The syngas processing (hydrocarbon synthesis from carbon monoxide and hydrogen) is a second stage of the most recycling processes of non-oil raw materials (coal, natural or associated gas, peat, etc.) to eco-friendly fuel components. Syngas processing is catalyzed by metals in bulk state or distributed on the surface of a highly porous support. Their catalytic activity, selectivity and stability is defined by the shape and size of the applied active component particles. Application of ultrafine catalyst systems allows the conversion reaction of synthesis gas with high efficiency in the traditional fixed bed reactors and in three-phase slurry reactors.

At synthesis of nanoheterogeneous contacts in liquid hydrocarbon medium nanosize stable suspensions with a size of particles no more than 50 nm are obtained. The disperse phase in such disperse systems isn't inclined to sedimentation that does them perspective for industrial realization in liquid-phase slurry -reactors.

At synthesis of nanoheterogeneous contacts distributed in solid organic matrix methods for polymer containing composite materials obtaining are used. Initial organic matrixes represent polyconjugated systems decomposing to carbon during formation of the catalyst. Thus particles of 10-20 nm in size metal are formed from salts immobilized on polymers.

Various physical-chemical methods of investigation of nanosized catalysts of synthesis gas conversion – IR- spectroscopy, magnetometry in situ, Mössbauer spectroscopy, X-ray diffraction, molecular modeling techniques will be described.

The work was carried out with the financial support of the Ministry of Education and Science of the Russian Federation.

Audience Take Away:

- The audience will learn about the current state of technologies for obtaining liquid hydrocarbons.
- The audience will learns about new types CO hydrogenation catalysts
- The audience will learn about the application of modern physico-chemical methods to the analysis of complex ultrafine (including molecular modeling)
- The audience working in the region will be able to apply new approaches to the synthesis of catalytic systems

Biography

Mayya Kulikova: 1974 year of birth; 1996 year – graduated from Federal State Budgetary Educational Institution of Higher Vocational Education «Gubkin Russian State University of Oil and Gas» with a degree in chemical engineering and ecology; 2000 year - passed PhD defense: «The synthesis of aromatic hydrocarbons from CO and H_2 in presence of bifunctional Co-zeolite catalysts» with degree in petrochemistry; 2000 – 2004 years - Assistant professor of faculty of Gas chemistry in Gubkin Russian State University of Oil and Gas; 2004 – 2008 years - Associate Professor of Inorganic Chemistry Faculty in Peoples' Friendship University of Russia; 2008 – 2014 years - Senior Researcher of A.V.Topchiev Institute of Petrochemical Synthesis, RAS (TIPS RAS); from 2014 to the present - Head of Catalytic synthesis department named by A. N. Bashkirov of A.V.Topchiev Institute of Petrochemical Synthesis Russian academy of sciences.

Efficient CO_2 hydrogenation to straight chain olefins over simple and robust alkali promoted Fe catalysts

Linga Reddy Enakonda*, Amol. M. Hengne, Lu Zhou, Kuo-Wei Huang, Jean Marie Basset
King Abdullah University of Science and Technology, Division of Physical Science and Engineering, KAUST Catalysis Center, Thuwal, Kingdom of Saudi Arabia

Use of carbon dioxide for the production of fuels and chemicals, which is widely emitted from fossil fuels on earth atmosphere and responsible for the greenhouse gas effect. Currently, utilization of carbon dioxide (CO_2) to various chemicals using homogeneous, heterogeneous, photo or electro-catalysts considered great importance both in industry and academics. As can be seen from the literature, there are many successful examples of commercial use of CO_2 to chemicals; for example use of CO_2 as feedstock in syn-gas for the production of methanol and dimethyl ether. Further investigation under consideration to develop active and selective catalysts for hydrogenation of CO_2 to synthetic fuels, light olefins, ketones, aldehydes and higher alcohols. The recent scenario on catalytic conversion of CO_2 to value-added chemicals and fuels has been considering as a very important objective, especially CO_2 hydrogenation for the production of lower olefins is highly important and challenging. Here, we develop efficient catalyst with single step preparation procedure, easy reducibility to metallic iron along with in-situ formation of active iron carbide species via methane activation at 750 °C for ‘x’ min (x=10 and 25 min) in a fluidized bed reactor, which are considered to be key steps for efficient activity and selectivity for FT process. Methane activation acts as a source of hydrogen, which is required for reduction iron oxide to metallic Iron. Here, our catalytic approach suggests that the efficient catalytic hydrogenation of carbon dioxide at temperature 250 °C with very high selectivity to olefins. At the same time, carbon source in terms multiwall CNTs obtained from the carbon of methane, which is key role for the formation iron carbide phases. Alkali promoted iron carbide catalyst possess efficient conversion of CO_2 about 28% with combined selectivity to light olefin (C2-C4), higher chain olefins (C5-C9) is about <55%.

Biography

Linga received Ph.D. in Chemistry from National Institute of Technology Trichy (India) in 2012. Before moving to KAUST, Linga worked as a Postdoctoral researcher from 2013 to 2015 with Prof. Dong Hyun KIM in the Chemical Engineering Department at Kyungpook National University, South Korea. In 2015, he moved to Prof. Jean-Marie Basset group at KAUST Catalysis Center in King Abdullah University of Science and Technology, Saudi Arabia. Linga research interests focus on catalysis and reaction engineering innovation for the conversion of fossil and biomass feedstocks to fuels and chemicals. Heterogeneous catalyst development for ultra-clean fuels production from fuel processing, CO_2 conversion and utilization; reforming of hydrocarbons and alcohol fuels for syngas and H_2 production; catalysis and reaction chemistry for energy conversion; and synthesis and applications of nano-porous catalytic and sorbent materials.

CONTENTS

Zirconium containing ionic materials as catalysts for C3, C4 alcohols conversions

Mikhalenko Irina Ivanovna*, Dr.Sc., Pylinina Anna Ivanovna, Ph.D., Povarova Elena Igorevna, Ph.D.
Physical and Colloidal Chemistry Department, RUDN University, Russia

Zirconium containing ternary phosphates $Na(Cs)_{1-2x}M_xZr_2(PO_4)_3$ (NASICON-family) and ternary oxides (vismuth vanadates $Bi_4V_{2-2x}Zr_{2x}O_{11-\delta}$ of perovskites family) in investigated series of compositions are studied for the vapor-phase selective dehydration and dehydrogenation of isobutanol and isopropanol in the temperature range 200-400 ^{0}C. These groups of catalysts represent the solid electrolytes (SE) with cationic and anionic conductivity respectively. The cations M(+2) = Co, Ni, Cu partially substitute the conducting ions Na^+ or Cs^+. For SE-catalysts characterization the methods XRD, XPS, IR, UVS, SEM, TEM, acidity/basicity surface titration were used. The results demonstrate the correspondence of NASICON frame structures for all of complex phosphates obtained, changes in surface composition vs bulk, different acid/basic sites in M presence and coordination of adsorbed alcohol molecule with hetero-linkages active site V-O-Zr in BIZRVOX. It is found the highest activity for a highly conductive γ-phase of BIZRVOX with selectivity 85–100% for isobutanal formation. The observed step-wise Arrhenius dependences for dehydrogenation reaction are related to changes in the conducting properties of the catalyst. The apparent activation energy decreases linear with phase transformation when Zr content increases. It is found that Cs-Zr-phosphates catalysts prepared by sol-gel procedure showed high selectivity in isobutene formation. But the nature of ion-dopant M as active site is very important too. We found the linear correlation between activation energy (Ea) for isopropanol dehydrogenation reaction (model reaction) and ionic radius of substituting ions M=Ni,Co,Cu in Na-Zr-phosphates prepared by solid phase synthesis. When temperature rises, the change in position M in conductive channel occurs and Ea value of alcohol dehydrogenation reaction diminishes. So, there are many examples confirming the relationship between conductive and catalytic properties of ionic's materials.

Audience Take Away:

- The collective properties of solid electrolyte catalysts as well as local composition of catalytic active sites must be taking into account in two reactions of C3-C4 aliphatic alcohols decomposing in anaerobic conditions producing olefin, aldehyde/keton and hydrogen.
- The results demonstrate the dependence of perovskites BIZRVOX catalytic activity on its crystal structure (zirconium content). Highly conducting anion-deficient phase is more active. NASICON type catalysts NZP family are perspective in H_2 and olefin producing with regulation of catalytic activity and selectivity by substitution of conducting Na(Cs) ions or frame zirconium ion.

Biography

Mikhalenko Irina I. graduated from Peoples Friendship University in 1974, PhD thesis defended in 1978 and a degree of Dr.Sci. in 1997 year. Research interests are adsorption and catalytic chemistry (reactions in vapor and gas phases, electro catalysis, photo catalysis). Led by I. Mikhalenko 9 graduate students, including 4 foreigners, have succeeded in PhD degree. At the Department of Physical and Colloidal chemistry I. Mikhalenko employs more than 40 years, has more than 200 publications, reads lectures in Physical chemistry, Colloidal chemistry, Nanochemistry, Thermodynamics of Nonequilibrium processes. Physico-Chemistry of surfaces and Chemisorption.

CONTENTS

Catalytic reduction of hazardous nitroaromatic groups

Halit Cavusoglu, Ph.D.
Selcuk University, Turkey

In recent years, green chemistry has gained significant attention to overcome the issue relating to the environmental contamination encountered by the worldwide population. The processes that prevent the use of organic solvents to convert harmful organic waste into low toxicity, reusable compounds in aqueous solutions under appropriate conditions are of great importance to scientists. In this context, recovery of nitrophenol (NP) compounds has been an important research area in recent times. The most common organic pollutants in industrial and agricultural wastewater are NPs. NPs are considered among the 126 priority pollutants and hazardous wastes by the United States Environmental Protection Agency (EPA) because of their high solubility in water, chemical stability, toxicity and persistence to environment and human health.

Catalytic reduction treatment technique has been introduced as a more sustainable method that can transform NPs into more eco-friendly products compared to other several advanced treatment techniques. More recently, various noble and transition metal nanoparticles including Au, Ag, Pt, Ni, Co, Cu, Ru and Pd nanoparticles have been widely used for the reduction of NPs as active catalysts. The size and shape of the preferred nanoparticles are very important parameters for their catalytic activity and selectivity in the chemical reactions. However, nanoparticles usually show low stability and such nanoparticles tend to aggregate because of their high surface energy. In order to solve this issue, it is a rational strategy to immobilize nanoparticles onto different appropriate supporting materials such as carbon-based materials (graphene, reduced graphene oxide), mesoporous silicas, metal oxides, and electrospun fibers.

Audience Take Away:

- This study can possibly be enlarged to other hetero-nanostructured materials, which are composed of noble metal nanoparticles (such as Pd, Pt, Ag and AuAg alloys) and metal oxide (such as ZrO_2 and V_2O_5) or carbon-based materials (graphene, reduced graphene oxide) supports. This kind of hetero-structured materials can be used in a wide range of implementations. In this context, researchers which focus on this field should expand their researches and teaching.

Biography

Halit Cavusoglu received his Ph.D. in Materials Science from the Selcuk University (2016). He spent ten years as a faculty member at Selcuk University with appointments in Physics and in Advanced Technology Research and Application Center. He is also managing director of a commercial company called “Grafenbiotech Nanotechnology Engineering Industry and Trade Company” in Turkey. He is conducting the company's research and development policy. His main research interests include design, fabrication, and characterization of thin-films, plasmonic and carbon-based nanomaterials.

Upgrading of furaldehydes via hydroxymethyration over heterogeneous acid catalyst

Shun Nishimura
Graduate School of Advanced Science and Technology, Japan Advanced Institute of Science and Technology (JAIST), 1-1 Asahidai, Nomi, Ishikawa 923-1292, Japan

Catalytic transformations of biomass resources towards value-added fuels/materials have attracted many research groups because the utilizations of these resources can contribute to the low CO_2 emission on the basis of carbon neutral concept and are sustainable/ renewable. Recently, we have focused on the upgrading of biomass-based C5 furaldehydes such as furfural and furfuryl alcohol towards the corresponding C6 furaldehydes (ex. 5 - hydroxymethylfurfural, 2, 5 - bis (hydroxymethyl) furan), through the direct hydroxymethyration reaction over various heterogeneous acid catalysts [Nishimura et al., under revision]. Previously, there are really few reports studying on similar transformations. In particular, Moreau and co-workers had undertook important discussions on this type of transformations [ex. Moreau et al., Ind. Crop. Prod. 9 (1999) 235]; e.g. approx. 10% yield for HMF production from furfural with the condition of formaldehyde/furfural = 240 was reported as the maximum value, however further improvement on the reactivity of heterogeneous catalyzed system is required.

Herein, we have examined two types of reactors with various heterogeneous acid catalysts; one is a conventional batch system and the other is a futural flow system. At present, it was observed that zeolite and commercial acidic resin of Amberlyst-15 gave significant performances for the hydroxymethylation of furfural to HMF with formaldehyde as a reagent; approx. 28% and 40% yields respectively were achieved in batch reactor. These values were much higher than that of previous achievements till 2017. It was worthy mentioned that the Amberlyst-15 catalyst was easily reusable over 4 runs in a batch reactor system and continuously produced HMF during 24 h in a flow reactor system. Moreover, Amberlyst-15 mediated hydroxymethyrations of other C5 furaldehydes such as furfuryl alcohol, furfurylamine and furoic acid were also proceeded.

In this presentation, I'd like to introduce the details of our recent studies and discuss the design of biomass conversions on the basis of this transformation.

Audience Take Away:

- The audience will find the rare but really important fundamental transformation of C5 to C6 furaldehydes.
- The audience will learn the importance/difficulty of the advanced flow reactor system application.
- We would share and discuss the futural design on biomass transformations.

Biography

SN is the Senior Lecturer in Japan Advanced Institute of Science and Technology (JAIST). He has completed his PhD (Materials Science) in March 2011, supervised by Profs. K. Ebitani and S. Maenosono. His research interests lie in the development of highly-functionalized nano-structured catalysts for productions of green energy and renewable materials. So far, he has published 50 refereed papers, 6 reviews/book chapters, 10 conference proceedings, and 14 patents application. He received the 2016 JAIST President's Award (Research Activity Award) in September 2016, and the Monthly Journal Award of the Bulletin of the Chemical Society of Japan (BCSJ) in March 2012.

DAY 1

POSTERS

2nd Global Conference on

Catalysis, Chemical Engineering & Technology

September 13-15, 2018
Rome, Italy

CONTENTS

Carbon nanotubes with tunable properties towards the design of efficient water denitration catalyst

Sanja Panic*, Ph.D., Goran Boskovic, Ph.D.
Faculty of Technology, University of Novi Sad, Serbia

Since their discovery in 1991, the unique tubular morphology of carbon nanotubes (CNTs) represents a great research challenge for many scientists over the world. The possibility of using different types of CNTs as catalyst support is still under extensive exploration. The process of water denitration is of great environmental significance. The catalytic reduction of nitrate to N_2 represents the efficient water remediation technique in terms of the achieved nitrate removal, but still with a main drawback – the production of ammonia as the undesired product. Thus, efforts are undertaken to solve the problem, in terms of both reactor and catalyst design. The application of chemically unmodified tubes for catalyst design has not received sufficient attention regardless of their initially different structural properties. The CNT defects originating from their preparation using various catalysts can be considered as a suitable substituent for subsequent deliberately formed anchoring sites on CNT surface by the functionalization process. Thus, the step in the catalyst preparation procedure that involves the use of strong mineral acids can be avoided, leading to simpler, cheaper and environmentally friendly way to synthesize the catalyst. In this regard, the aim of this work was to synthesize various Pd-Cu/CNT denitration catalysts using multiwalled carbon nanotubes (MWCNTs) of different structural quality, evaluate the influence of their surface chemistry on the metal active phase characteristics and, consequently, test their performances in water denitration reaction. Water denitration is a structure sensitive reaction related to Pd particle size, and this effect is further emphasized in the decoration of the particle by the incorporation of Cu atoms into Pd particle corners and edges. The extent of lattice defects in CNTs was found to dictate the size and composition of the Pd-Cu active phase, playing an important role in nitrate reduction. Catalyst samples characterized by close proximity of Pd and Cu, as in an alloy, displayed the highest degree of nitrate conversion. At the same time, the size of the Pd particles, alone, or decorated to different extents with Cu atoms, was found to be critical for the second step of denitration reaction, directing the formed nitrite to either N_2 or NH_3.

Audience Take Away:

- Detailed analysis of Pd-Cu/CNT catalysts used for water denitration;
- The catalyst performances can be tuned by the application of CNTs of different degree of lattice defects as catalyst support;
- Insight into the effect of Pd particle size and bimetallic particle composition;
- Confirmation of the structure sensitivity effect of water denitration reaction.

Biography

Ph.D. in Technology Engineering, scientific discipline Chemical Engineering – Catalysis (2014), Faculty of Technology, University of Novi Sad, Serbia;

M.Sc. in Pharmaceutical Engineering, Faculty of Technology, University of Novi Sad, Serbia (2004);

More than 10 years of research experience in the field of heterogeneous catalysis - optimization of carbon nanotubes synthesis by CVD method over different catalysts, CNTs purification methods, potential applications of CNTs in the field of environmental protection – as adsorbents and support for new heterogeneous catalysts;

Publications: 1 book chapter, 13 peer-reviewed journal articles, 2 conference publications – full paper reviewed, 24 conference publications – abstract reviewed, citations 56 (including selfcitations), cumulative impact factor 31.47, h-index 4;

Reviewer for Journal of Materials Research, Reaction Kinetics, Mechanisms and Catalysis, Processing and Application of Ceramics, Environmental Pollution, Applied Catalysis A – General

Ni^{2+} and Ni^+ counterions in MFI zeolite as single and multiple coordination sites for small molecules

Elena Zdravkova Ivanova[1]*, Ph.D., Videlina Zdravkova[1], Mihail Mihaylov[1], Ph.D., Konstantin Hadjiivanov[1], Hristiyan Aleksandrov[2], Ph.D., Petko Petkov[2], Ph.D., Georgi Vayssilov[2]
[1]Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, Sofia 1113, Bulgaria
[2]Faculty of Chemistry and Pharmacy, University of Sofia, Sofia 1126, Bulgaria

A relatively new field in heterogeneous catalysis is aiming at developing catalysts formulation where platinum group metals are replaced by more abundant and cheap 3d base metals for industrial and environmental adsorption and catalytic applications. An important requirement for such systems is that the 3d metal is in the form of coordinatively unsaturated (CUS) cation state having the proper energetics for adsorption and/or catalytic transformation of molecules. The stabilization of such state can be achieved when cations are ion-exchanged in zeolite structures. A very suitable analytical method to study the CUS-state of cations is IR spectroscopy of probe molecules.

In this presentation we summarize our extensive work on IR studies of adsorption of probe/guest molecules such as CO, NO, N_2, O_2, H_2O along with isotopically labeled molecules to determine the state of Ni cations in ZSM-5 zeolite The IR studies are combined with density functional theory (DFT) modeling to justify the assignment of vibrational modes of adsorbed molecules and thus to prove the state of metal.

Ni^{2+} ions in the ZSM-5 matrix are highly electrophilic due to their low coordination. The theoretical calculations find that the Ni^{2+} ions are coordinated to four zeolite oxygen centers. As a result Ni^{2+} forms relatively stable monoligand complex with NO, CO and N_2. The binding energies (BE) of these ligands calculated by DFT are -173, -112 and -57 kJ/mol, respectively.

Another consequence of the low coordination of Ni^{2+} cations in ZSM-5 is their ability to coordinate two small molecules. Our theoretical prediction find preferential formation of $Ni^{2+}(NO)_3$ and $Ni^{2+}(CO)(NO)_2$ to occur. The IR experiments, however, reveal the formation of $Ni^{2+}(NO)_2$ and $Ni^{2+}(CO)(NO)$ complexes.

Ni^+ ion has larger ionic radius than Ni^{2+} and our DFT calculations showed that Ni^+ ions are bonded to two O atoms of the zeolite. As a result Ni^+ can bind up to tree CO molecules. BEs of successively added CO molecules are calculated to be -168, -94, and -26 kJ/mol. The Ni^+-CO species are much more stable as compared to Ni^{2+}–CO because of the formation of a π bond and the synergism between the σ and π bonds. All monocarbonyls can be converted into dicarbonyls but even at low temperature and high CO pressure, di-carbonyls are not completely converted into tricrabonyls, likely due to the existence of steric restrictions for specific positions Ni–ZSM-5 channels. Ni+ ions are able to form $Ni^+(N_2)_2$ complexes. The latter can lose their ligands stepwise, producing two types of linear Ni^+–N_2 species. Calculated BE of the first and the second N_2 ligand is -86 and -27 kJ/mol. As predicted by DFT calculations, formation of mixed ligand $Ni^+(CO)(N_2)$ complexes is observed by IR. Complexes with NO ligands are not experimentally registered even at low temperatures as Ni^+ is spontaneously oxidized by NO to Ni^{2+}. No mixed ligand complexes of Ni^{2+} and Ni^+ with aqua ligands are observed.

Audience Take Away:

- The ZSM-5 zeolite provides unique extra-framework sites where the exchanged Ni cations are in low coordination state and can attach more than one guest molecule. In addition, the ZSM-5 structure is able to stabilize a non-trivial oxidation state for nickel, i.e. the Ni^+ cationic state. These facts signify the advantages of ZSM-5 as a host for nickel cations as compared to other host systems and make the Ni-ZSM-5 system a promising material for adsorption and catalytic applications.
- Fundamentals of the formation of geminal and mixed-ligand complexes of gas molecules on the surfaces and its relation to adsorption and catalysis will be highlighted.
- This presentation will help researchers from materials and catalysis branches to use IR spectroscopy of probe molecules for characterization of metal sites in porous materials. In additions, the use of isotopic probe molecules for identification of geminal complexes will be exemplified.

CONTENTS

Biography

Elena Ivanova studied Chemistry at the Sofia University (Bulgaria) and graduated as MS in 1999. She then joined the research group of Prof. K. Hadjiivanov at the Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences (IGIC-BAS). She received her PhD degree in 2004 at the same institution. After one year postdoctoral fellowship supervised by Dr F. Thibault-Starzyk at the Catalysis and Spectrochemistry Laboratory (LCS) (Caen, France), she obtained the position of an Associate Professor at the IGIC-BAS.

In-situ imaging of electrolyte flux in a Li-ion battery

Keiji Takata
Faculty of Engineering Science, Kansai University, 3-3-35 Yamate-cho, Suita, Osaka 564-8680, Japan

Li-ion batteries have advantages including high energy density, high output voltage, and the absence of the memory effect, and so are recognized as promising candidates for energy storage.

Li-ion batteries operate through the migration of Li ions between the electrodes. Therefore, non-destructive observation of the migration with high spatial resolution is important.

Layered materials are commonly used as electrode materials for Li-ion batteries. When charging and discharging, Li-ions are extracted or inserted into the interlayers, which causes changes in volume. Scanning probe microscopy (SPM) can allow high resolution imaging of these volume changes, which enables us to investigate Li-ion migration without destruction. Here, we present our results of $LiCoO_2$ cathodes in Li-ion batteries.

The active materials in the electrodes were layered $LiCoO_2$ and graphite, which are commonly used in the batteries. Li-ions migrated between $LiCoO_2$ and the graphite during the charging/discharging cycle, which led to changes in the volume of the active materials. SPM is capable of imaging properties inducing strains in a sample non-destructively and with a high spatial resolution.

Volume changes of $LiCoO_2$ generated by Li insertion/extraction are very small, 10-2, and so they hardly appeared in our obtained images. However, the $LiCoO_2$ particles were imaged as dark portions with no signal as shown by (b), because changes in volume in the interspace were detected. We concluded that electrolyte flux induced by the gradient of Li-ion concentration in the cathode caused the volume changes in the interspace. Graphite or silicon yields large volume changes by changing/discharging, which induces electrolyte flux. This often causes dry-out of electrolyte. In the case of $LiCoO_2$, the concentration gradient of Li ions induced the electrolyte flux.

This electrolyte flux is one of the most important issues for increasing the energy density of lithium ion batteries.

Audience Take Away:

- Our presented method is a powerful tool for research & development of the Li-ion battery. Great advances in the research & development should be achieved.
- Our method is very simple and easy. Anyone can try it.
- We presented fruitful results for development of the Li-ion battery. Manufacturer can achieve great improvements of the batteries using our results.

Iron hydroxide-based adsorbent: A case study in removing of H_2S from biogas

Edoardo Magnone[1]*, Shin Dong Kim[2] and Jung Hoon Park[1]
[1]Dongguk University, Department of Chemistry & Biochemical Engineering, Manhae gwan - Room B215 - 30, Pildong-ro 1gil, Jung-gu, 100-715, Seoul, Republic of Korea
[2]E&Chem Solution Corporation, Energy & Environment R&D Center, Pocheon-si, South Korea

Methane (CH_4) - an important energy source - is the main component of the biogas generated in a Landfill-Based Anaerobic Digestion (LBAD) process but its use in practice is still dependent upon the presence of hydrogen sulfide (H_2S). This study was aimed to evaluate the H_2S removal efficiency of an economic iron hydroxide-based adsorbent from simulated biogas mixture. The properties of these porous materials such as crystal structures, surface patterns, surface area, pore volume and pore size were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and BET measurements. Its adsorption capacity was systematically measured as a function of drying temperature conditions, and the process variables like space velocity, retention time, relative humidity as well as the H_2S concentrations. In summary, the results obtained from this study are indicated as follows: (i) the behavior of iron hydroxide-based adsorbents for removal of H_2S from simulated digester gas mixture does not depend on the drying temperature treatment of samples and relative humidity of the inflow biogas. (ii) H_2S removal efficiency increases as H_2S concentration increases. This means that the very versatile properties in the different H_2S concentration of iron hydroxide-based adsorbents make possible their application with a wide range of biogas and, in addition, they are very effective adsorbent for high-concentration H_2S-containing processes.

Audience Take Away:

- This Poster Presentation promising in the field of separation techniques using mesoporous adsorbents and the topic related to the application of iron hydroxide-based adsorbents in separation technology for removal of H_2S from biogas and then environmental protection.

Biography

Magnone graduated in Chemistry at the Institute of Physical Chemistry, University of Genoa. In 1999 he received his Ph.D. degree in Chemical Science at the Department of Chemistry and Industrial Chemistry, University of Genoa, with a bias in his research toward the chemistry, electrochemistry, materials science and closely related fields. In 2004, he moved to the Research Centre for Advanced Science and Technology (RCAST) at the University of Tokyo where he served as visiting research associate before at the Department of Applied Chemistry (2004-2008) and then Komaba Open Laboratory (2008-2009). He has also served as research associate at the WPI - Centre for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS) in Japan (2009-2010) and the Korea Institute of Energy Research (KIER) in Korea (2010-2013) as a researcher in the field of membrane science as well as nanomaterials synthesis and processing for high-performance applications. At present Magnone is serving as assistant professor in the Department of Chemistry & Biochemical Engineering, Dongguk University, Seoul (Korea).

Use of Cu^I-ZSM-5 for purification of the fuels of the future (Methane and Hydrogen)

Mihail Yordanov Mihaylov*, Ph.D., Kristina Chakarova, Ph.D., Nikola Drenchev, Ph.D., Konstantin Hadjiivanov
Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria

Hydrogen and methane are often considered as principle fuels of the future. Hydrogen is the most environmentally friendly fuel because its burning does not pollute the environment. Methane is next to hydrogen as CH_4 emits less CO_2 upon burning than other hydrocarbon-based fuels.

Some technological applications require a high purity of fuels. For example, fuel cells require hydrogen feed to contain less than 10 ppm CO in order to avoid catalysts poisoning. Removal of N_2 from natural gas is essential to achieve efficient utilization of CH_4 (e.g., to meet the requirements of pipes).

Adsorption-based technologies for purification of gases have attracted increased interest because of their energy efficiency. These technologies have the potential to achieve high selectivity in gas separation processes that need to be further developed and optimized.

In this presentation Cu^I-ZSM-5 will be considered as an adsorbent material for obtaining high quality H_2 and CH_4 gases free from impurities like CO and N_2. Cu-ZSM-5 samples are prepared by conventional aqueous and solid state ion exchange (SSIE) of H-ZSM-5 with Cu^{II} and Cu^I ions, respectively. In the former case, Cu^{II} ions need to be reduced to Cu^I state, while in the latter Cu^I ions are directly inserted in the zeolite matrix by using a CuCl salt. In this study, the reduction of Cu^{II} in Cu-ZSM-5 material is achieved by CO, as followed by temperature-programmed reduction (CO-TPR). The adsorption properties of the samples are further characterized by in situ FTIR spectroscopy, pulse adsorption and temperature-programmed desorption of CO (CO-TPD). We find in this work, that CO strongly binds to CuI sites forming Cu^I-CO complexes; these complexes can be destructed at high temperature. Studying $^{15}N_2$ adsorption, we observed formation of Cu^I-$^{15}N_2$ complexes and most of the CuI sites are occupied at low pressure; N_2 is removed after prolonged evacuation at room temperature (RT). The effects of water vapor and O_2 on the adsorption of CO and N_2 are also studied by FTIR. In the presence of O_2, the CuI state is stable up to 100oC. Addition of H_2O vapor to the system with pre-adsorbed CO leads to formation of $Cu^I(CO)(H_2O)_x$ complexes, which can be back converted to Cu^I-CO species upon outgassing at RT. N_2 adsorption is hardly affected by H_2O at low levels of humidity. The adsorption of H_2 and CH_4 is much weaker and practically take place only at low temperature. Finally, the potential of materials for gas adsorption/separation processes is verified by pulse technique and TPD. Under flow conditions, CO can effectively be captured at RT, while N_2 is caught at water freezing temperature. Using the SSIE method, materials with almost completely exchanged protons are achieved. Thus, high number of Cu^+ sites active for CO and N^2 adsorption is obtained, while acid OH groups active for adsorption of both N_2 and CH_4 are eliminated.

Audience Take Away:

- The adsorption of CO on Cu^I-ZSM-5 by forming Cu^I-CO species is very strong. The process is hardly affected by O_2 and H_2O under ambient conditions. Therefore, Cu^I-ZSM-5 based materials can be used as adsorbents for fine purification of H_2 from CO impurity. Although the energetic difference between CH_4 and N_2 adsorption on Cu^I-ZSM-5 is smaller, the material seems to show potential for CH_4/N_2 separation as well.
- The adsorption behavior of Cu^I-ZSM-5 material may be controlled by the preparation method. High metal-to-proton exchange levels for Cu^+ ions can be achieved by the application of solid state ion exchange (SSIE) method. However, materials obtained by SSIE method usually contain occlusions of CuCl and Cu_2O that can hinder the gas purification/separation capability.
- This poster presentation will highlight the power of IR spectroscopy to study the materials performance in gas adsorption/separation and detection applications.

Biography

Mihail Mihaylov studied Chemistry at the Sofia University and graduated as M.S. in 1997. Receiving his Ph.D. degree in the field of spectroscopic methods in catalysis in 2003, he continued his work under the supervision of Prof. Konstantin Hadjiivanov at the Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences (IGIC-BAS). In 2007, as a Humboldt Foundation fellow he completed a research program on gold catalysis in the group of Prof. Helmut Knözinger at the University of Munich (LMU). Since 2008, MM is Associate Professor of chemistry at the IGIC of BAS. He has coauthored 66 scientific papers in peer-reviewed international journals. His research is mainly focused on fundamental studies of adsorption and catalysis phenomena on oxide and metal-oxide surfaces by the application of FTIR spectroscopy.

Composite thin films based on Zno - carbon derivatives for photocatalytic applications

Dana Perniu*, Maria Covei, Cristina Bogatu, Anca Duta
R&D Centre, Renewable Energy and Recycling, Transilvania University of Brasov, Romania

Now-a-days photocatalysis is widely recognized as efficient for pollutants removal, but the largescale application still face challenges. One of the most prominent challenges is the use of photocatalysts (e.g. TiO_2, ZnO, etc.) that are activated under UV radiation, which implies additional costs. The need to extend the activation spectral range to the visible region is mainly met by semiconductor doping or coupling with other materials such as other semiconductors, noble metals, and most recently, carbon-based derivatives. The development of photocatalysts usually require expensive, energy intensive processes (sputtering, hydrothermal, etc.), increasing thus the overall costs of the application.

In this context, the photocatalyst approached in this paper is a composite-type material answering to the need of improved photocatalytic effect under combined UV+VIS radiation (simulated solar radiation) consisting of ZnO and carbon derivatives, obtained as thin films by spray pyrolysis deposition, as novel method for this application.

The effect of the zinc precursor (zinc chloride or zinc acetate), of the type and amount of the carbon derivatives (graphene oxide and reduced graphene oxide) and other additives (surfactants, polymers, etc.), as well as the deposition parameters on the thin film properties is discussed. Particular attention is payed to the morphology of the thin films, which is essential to the adsorption stage in the photocatalytic process.

The photocatalytic efficiency of the thin films on the degradation of organic pollutants such as methylene blue and phenol, under solar simulated radiation is presented. The effect of carbon derivatives addition to the oxide thin film is highlighted and is correlated to the effect of thin film morphology and chemical composition. Photocatalytic efficiency, alongside thin film wettability are considered for the purpose of selecting the most promising composite for self-cleaning.

Audience Take Away:

- Spray pyrolysis deposition as novel synthesis and deposition method for ZnO – Carbon derivatives composite thin films.
- The key requirements that govern the synthesis of this type of thin films with controlled surface properties.
- The photocatalytic performance of these thin films, in relation to the films' surface properties.
- The presentation outline the design requirements for developing composite thin film materials targeting large scale applications.

Biography

Dana Perniu is professor in the Transilvania University of Brasov, and member of the Research Center Renewable Energy Systems and Recycling. The research activity is focused on materials for solar energy conversion: oxide materials for development of colored solar thermal collectors, ternary and quaternary semiconductor materials for solar cells ($CuInS_2$, $CuSbS_2$, Cu_2ZnSnS_4), oxide (TiO_2, ZnO) and coupled semiconductors ($TiO_2/Cu_xS/Ag$, TiO_2/ Cu_2ZnSnS_4) as VIS-active photocatalyst for organic pollutants removal (dyes, chemical warfare agents).

Fabrication and characterization of perovskite catalyst for oxygen removal in landfill gas (LFG)

Edoardo Magnone, Jin Woong Chae, Jung Hoon Park*
Dongguk University, Department of Chemistry & Biochemical Engineering, Wonheung-gwan F619, 30, Pildong-ro 1gil, Jung-gu, Seoul, 100-715, Korea

In recent years, the purification of landfill gas (LFG) to produce pipeline-quality gas has attracted increased research interest also due to its crucial role in producing energy or other products. At present, the vast majority of catalytic deoxygen catalyst materials for the reduction of O_2 in the LFG are Pd-, Pt, and Rh-based noble metals of various compositions. In this work, the perovskite-type oxides with general formula $La_{1-x}Sr_xCo_{0.2}Fe_{0.8}O_{3-d}$ (x=0.1-0.9) are proposed as advanced methane oxidation catalysts for the deoxygen technology of LFG at intermediate temperature with the aim to reduce the use of precious and noble metals. The hollow fiber type catalyst with o.d. 1.4 mm/ i.d. 0.7 mm/10 mm length was prepared and tested in a lab-scale oxygen removal equipment under various temperature and feed conditions. The total oxygen conversion was confirmed at 475ºC and it was maintained over 100 hours in a long-term test.

Audience Take Away:

- The high-performance and durability test results obtained in this work by perovskite-type oxides with general formula $La_{1-x}Sr_xCo_{0.2}Fe_{0.8}O_{3-d}$ (x=0.1-0.9) are promising and represent an important step towards the successful implementation of new LFG deoxygen treatment technologies.

Biography

Dr. Park studied his bachelor (1988/1993), master's degree (1996/1994) and Ph.D. (1996/2000) at the Department of Chemical Engineering of the Korea University, Seoul (Korea). From 2000 to 2013 he was a researcher at the Korea Institute of Energy Research (KIER), Daejeon (Korea). Actually, Dr. Jung Hoon Park is an Assistant Professor at the College of Engineering of Dongguk University in Seoul (Korea) and team leader of a laboratory specialized on Carbon capture and storage (CCS). His activity focuses on oxygen separation using ion transport membrane as well as hydrogen separation using metal and ceramic composite membrane, fine ceramic synthesis using hydrothermal reaction, and supercritical water extraction.

Formation of catalytic active cites in Copper modified Ce-Mn mesoporous oxides for ethyl acetate total oxidation

Radostina Nikoaleva Ivanova*, Ph.D. student, Gloria Issa, Ph.D., Momtchil Dimitrov, Ph.D., Tanya Tsoncheva
Institute of Organic Chemistry with Centre of Phytochemistry, BAS, Bulgaria

Volatile organic compounds (VOCs) are recognized as major contributors to air pollution due to their toxicity to human health and the formation of photochemical smog. Nowadays, the increasing political, social and economic attention on the environment and the quality of life has enforced the strict monitoring of VOCs emissions and the development of efficient technologies for their elimination. The catalytic total oxidation has been recognized as more economic process even when VOCs were emitted in low concentrations. Due to the relatively low price and stability to various poisons, the transition metal oxides could be more efficient catalysts compared to noble metals. A well-known approach to improve their catalytic activity is the preparation transition metal oxides in the nanoscale. Our previous study showed good catalytic activity of the mixed cerium-manganese oxide system in the studied reaction. There are few reports showing that the addition of copper to CeMnOx favors the catalytic activity in oxidation processes. The aim of the current investigation is development of new nanostructured mesoporous metal oxide systems based on ceria-manganese oxides promoted with copper (CuMnCeOx) and their application as catalysts in ethyl acetate total oxidation. The influence of the preparation procedure of ceria-manganese oxide supports on the state of copper will be followed in detail.

Biography

Radostina Ivanova is PhD student in Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Science, lab." Organic Reactions on Microporous Materials". The results of her work are formed in 24 publications, 12 of which in scientific journals with a high impact factor. She has participated in 25 international scientific conferences with oral and poster presentations.

Hydrogen evolution over Gallium oxynitride prepared from Gallium oxide hydroxide under visible light irradiation

Yuma Kato*, Muneaki Yamamoto, Ph.D., Akiyo Ozawa, Tetsuo Tanabe, Ph.D., Tomoko Yoshida Ph.D.
Osaka City University, Japan

We study water splitting reactions using solid photocatalysts. It is well known that only 6% or less energy of sunlight is given by UV light, while more than 50% by visible light. Therefore, it is important to prepare photocatalysts driven by the visible light for the efficient use of the sunlight energy. Recently, it has been reported that nitrogen doping into metal oxides contributes to narrowing of their band gap, providing a visible-light response because N 2p orbitals are newly formed above O 2p orbitals in their valence band. To generate visible light response in gallium oxide (Ga_2O_3) photocatalysts, which showed high photocatalytic activities of water splitting reaction under UV light irradiation, we have tried nitrogen doping into Ga_2O_3. However, under visible light irradiation, gallium oxynitride (referred as GaON) prepared from Ga2O3 did not show the activity even for hydrogen evolution from methanol aqueous solution. In this study, GaON samples were prepared by calcination of gallium oxide hydroxide (GaOOH), a precursor of Ga_2O_3, under NH3 atmosphere at 773-1173 K. The prepared photocatalysts were characterized by Field Emission-Scanning electron microscopy (FE-SEM), UV-vis diffuse reflectance (DR), powder X-ray diffraction (XRD), X-ray absorption fine structure (XAFS) and X-ray photoelectron (XP) spectroscopies to analyze their optical properties and crystalline structures.

N K-edge XANES spectra showed that prepared GaON samples contained nitrogen after nitrogen doping. The spectral profiles represented the chemical states of doped nitrogen, i.e., molecular nitrogen existed as interstitials when nitrogen doping temperature was under 973 K and above 973K gallium nitride (GaN) precipitated. However, radial structure functions of Ga K-edge EXAFS spectra of the samples were not strictly consistent with that of commercially available GaN, suggesting that some Ga-O bonds is remained. H2 evolution reactions from methanol aqueous solution using prepared samples were performed under visible light irradiation (λ>420 nm). This reaction did not proceed over commercially available GaN and prepared samples except the sample prepared at 1173 K. In order to understand why such difference in photocatalytic activity appeared, we investigated XRD patterns before and after the reaction. We found that bulk crystalline structure of the sample prepared at 1173 K fundamentally maintained while those of others had changed probably due to release of doped nitrogen. In this conference, we would like to discuss this topic in detail and ask you to give some advises to us.

Audience Take Away:

- In our laboratory, various solid photocatalysts have been prepared by a lot of synthesis methods and their photocatalytic activities for water splitting or CO_2 reduction have been examined in detail. In this study, we will provide a new synthesis method for nitrogen doping into solid photocatalysts.
- In order to investigate the chemical states and crystalline structures of prepared photocatalysts, we performed a lot of characterization such as UV-vis diffuse reflectance, FE-SEM, TEM, XRD, XRF, XPS, XAFS, in situ FT-IR and electrochemical measurements by ourselves. The audience will understand that the above characterization techniques are very useful for the optimal designs of photocatalysts.
- In addition to the preparation and analysis of solid catalysts, we are trying to calculate the electronic structure of the solid photocatalysts using a first-principle calculation method based on the density functional theory (DFT). We can also provide knowledge and skills on theoretical calculation.

Biography

Yuma Kato got a bachelor of engineering at Osaka City University (Japan) in 2017. Now, he is a graduate student of engineering at Osaka City University. He is currently working on developing Ga2O3 photocatlyst to use for CO_2 reduction under visible light irradiation. He got a poster prize at 9th OCARINA International Symposium in 2018.

Spectroscopic investigation of the influence of UV-irradiation on hydroxyl-hydrated layer of TiO_2 photocatalyst

Ekaterina A. Toscheva, Aida V. Rudakova Ph.D., Kirill M. Bulanin*, Ph.D.
Saint-Petersburg State University, Russia

Applications to environmental cleanup have been one of the most significant areas in heterogeneous photocatalysis for a long time. Titanium dioxide is the most widely used photocatalyst, which provides the most reasonable trade-off between photocatalytic performance, stability in broad variety of chemical environments, low price, and essential low toxicity.

FT-IR spectroscopy is well known as useful technique for study of adsorbed species. This method is especially sensitive to water molecules and superficial OH-groups, though the spectral line broadening due to H-bonding (in the case of high surface coverage) makes the interpretation somewhat difficult.

In our experiments, powdered samples were pressed into the self-supported pellets with the thickness of about 0.1 mm, and outgassed at elevated temperatures in vacuum followed by the annealing in the presence of oxygen for removal of organic impurities. Then, experiments were carried out at ambient temperature.

In present work, the influence of UV-radiation applied to powdered TiO_2 samples was investigated spectroscopically under vacuum conditions (~3E-6 torr). Experiments were performed in-situ at different stages of surface hydration for simulation of the case of superhydrophylic self-cleaning films at ambient conditions. Surface species formed were detected and analysed. Mechanisms of the hydroxy-hydrated layer reconstruction being under the action of UV-Vis radiation were considered.

Audience Take Away:

- Knowledge of applications of the FT-IR Spectroscopy method coupled with specially designed experimental set-up that is very effective in in-situ as well as ex-situ investigations of photoprocesses on such a complicated systems as powdered catalysts.
- Presented technique can be used for in-situ investigation of broad variety of powdered systems and thin films.
- Results obtained show that this is the area which other researchers could use to expand their research in the field of heterogeneous catalysis.
- This experimental approach gives investigators the effective practical solution for in-situ as well as ex-situ spectroscopic studying of heterogeneous systems.

Biography

Kirill M. Bulanin has got his PhD degree in 1997 at the University of Caen (France) on the Physical chemistry topic, focusing the spectroscopic studies of surface species. He spent 6 years at the University of Delaware (USA) as a Post-Doctoral fellow working at the Chemical Engineering Department, and the Department of Chemistry and Biochemistry. Also, he spent 2 years working at R&D department at the Samsung SDI Company (South Korea). Currently, he works as a lecturer (docent) at the Department of Physics, Saint-Petersburg State University, Russia, and as a senior researcher at the Laboratory of Photoactive Nanocomposite Materials.

CONTENTS

Graphene Oxide supported Tio$_2$ nanocomposites

Ayşe Neren Ökte*, Duygu Tuncel
Boğaziçi University, Turkey

TiO2 is the most extensively used photocatalysts in the advance oxidation processes owing to their complementary psychochemical properties, low cost, non-toxicity and high efficacy. However, poor adsorption capacity, formation of rapid aggregates in suspension systems and recycling problems limit the utilization of bare TiO$_2$. Higher specific surface area and more effective adsorption sites are being elucidating advantages of using supported catalysts. The enhanced degradation rates can be attributed to the increased condensation of pollutants on the supported catalysts by adsorption and the reduced electron-hole recombination process on the surface. Therefore, in practical applications, attempts have been made to use porous adsorbent materials for supporting catalyst nanoparticles.

Graphene is a two-dimensional material, composed of single-, bi- and few- (≤10) layers of carbon atoms forming six-membered rings. In recent years, graphene-related materials have been used in the adsorption processes due to the large surface area and ordered layered structure. In addition, graphene oxide possesses the ability to accept the electrons from semiconductors and to prevent recombination of photo generated electrons and holes.

In this study, graphene oxide supported TiO$_2$ nanocomposite is synthesized and characterized by using X-Ray Diffraction (XRD) Analysis and Scanning Electron Microscopy with Energy Disperse X-Ray Analysis (SEM-EDX). Photocataytic activity of the composite is examined for the decolorization of methyl orange (MO) under UV irradiation.

Audience Take Away:

As preliminary experiments and baseline information:

- Determination of photocatalytic activities of the TiO$_2$ supported grapheme.
- Determination of physico-chemical properties of the supported catalyst.

Understanding of the physico-chemical behavior of the reacting partners:

- Application of specific physico-chemical methods, i.e. surface area and pore size distribution, particle size calculations, absorption properties etc.
- Application of novel photocatalysts in adsorption and photocatalytic degradation systems.

Biography

A.Neren Ökte is a Professor of Physical Chemistry in Boğaziçi University. Her research interests cover physical and material chemistry, in particular, photocatalysis, supported catalyst systems, transition and inner transition metal-ion loaded photocatalysts, kinetics and photochemistry.

CONTENTS

$CaAg_2$ as catalyst precursor for ethylene epoxidation

Antonyshyn Iryna*[1], Sichevych O.[1], Rasim K.[1], Ormeci A.[1], Burkhardt U.[1], Titlbach S.[2], Schunk S. A.[2], Armbrüster M.[3], Grin Yu[1]
[1]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany
[2]hte GmbH, Kurpfalzring 104, 69123 Heidelberg, Germany
[3]Faculty of Natural Sciences, Institute of Chemistry, Materials for Innovative Energy Concepts, Technische Universität Chemnitz, 09107 Chemnitz, Germany

Ethylene oxide (EO) is one of the target products for chemical industry. The supported and promoted silver is nowadays used as catalyst for ethylene epoxidation process using molecular oxygen. In order to enhance the selectivity towards ethylene oxide instead of thermodynamically favorable carbon dioxide (CO_2) and water (H_2O), the development of efficient catalysts is crucial. Numerous studies on epoxidation reveal that the electronic structure of the catalyst surface layer has a tremendous impact on the adsorption properties of reactants and the nature of reaction intermediates. Bimetallic catalysts (e.g. Ag–Cu, Ag–Pd) were assumed to be useful systems for tuning of catalytic activity with electronic structure. However, their advanced investigation under reaction conditions affirms that the surface changes drastically during the epoxidation and the reaction mechanism is governed by the state of the surface. The chemistry of such catalyst systems is highly dynamic and not trivial. In contrast, intermetallic compounds (IMCs) due to their ordered crystal structure can be useful model systems for understanding the catalysts' behaviour under reaction conditions.

The binary compound $CaAg_2$, one of the binary compounds in the system Ca–Ag with well-defined and ordered crystal structure, was tested as a catalyst for ethylene epoxidation. The conversion and selectivity towards EO increase during the induction period and afterwards remain stable for several hundreds of hours.

Based on PXRD and SEM analyses as well as calculations of adsorption energies of oxygen atoms at different partial pressures, the presence of more electronegative oxygen in the atmosphere (gas stream) and high affinity of calcium to oxygen lead to formation of calcium oxide and a significant segregation of silver to the surface. In addition, presence of carbon dioxide and water vapour from the unwanted total combustion leads to a variety of possible Ca-related products of $CaAg_2$ oxidation, e.g. CaO, $Ca(OH)_2$ and $CaCO_3$. The oxidation of pristine $CaAg_2$ towards elemental Ag is accompanied with formation of a porous 3D microstructure of intermediates and Ca-containing oxidation products. This microstructure is remarkably stable and prevents further sintering of the silver particles. The comparison of in situ formed Ag catalyst (using $CaAg_2$ as precursor) with an Ag/CaO catalyst (prepared using a classical impregnation method) reveals the unique catalytic behaviour of the Ag-based catalyst obtained during $CaAg_2$ oxidation.

Audience Take Away:

- Investigation of new catalytic system enhances our knowledge about the catalyst behaviour under epoxidation conditions;
- They highlight the advantages of using intermetallic compounds with well-defined crystal structure as precursor for synthesis of Ag-based catalysts;
- An interrelated understanding of crystal and electronic structures as well as chemical bonding of IMC can be a powerful tool for future catalyst development and/or optimization.

Biography

Iryna Antonyshyn studied chemistry at Ivan Franko National University of Lviv (Lviv, Ukraine) and received her diploma in 2006. In 2006–2011 the scientific work on PhD thesis "Interaction of gallium and antimony with transition (V, Mn) and rare-earth (Y, La, Ho) metals" under supervision of Dr. Stepan Oryshchyn was carried out. During this period she earned DAAD scholarship and joined the group of Prof. Juri Grin in Max-Planck Institut für Chemische Physik fester Stoffe (Dresden, Germany) for 10 months (2008–2009). After successful PhD defense in 2011 she joined the same group as postdoc. The main topic of her research is chemical properties of intermetallic compounds and their application in the field of heterogeneous catalysis.

CONTENTS

Comparative study of self-cleaning properties of TiO_2, ZnO-based photoactive materials

Aida Rudakova[1]*, Ph.D., Maria Sivokhina[2], Anastasia Laptenkova[3], Petr Murzin[4], Ph.D.
[1]Senior Researcher, Head of the Division ”Synthesis of Photoactive Materials”, Laboratory of Photoactive Nanocomposite Materials, Saint-Petersburg State University
[2]Bachelor's student, Department of Physics, Saint-Petersburg State University
[3]Graduate student, Department of Chemistry, Saint-Petersburg State University
[4]Department of Physics, Saint-Petersburg State University

Self-cleaning materials have considerable attention for both their unique properties and practical applications in energy and environmental areas. Self-cleaning properties of such materials include photocatalytic activity, ability to photoinduced superhydrophilic transition, and bactericidal acting. Vigorous applied studies of the effect have resulted in the development of self-cleaning and anti-fogging glass, self-cleaning coating for exterior and interior surfaces for windows, buildings, tunnels, road shields and, so on. Concerning mechanisms of photoinduced processes, no doubt that the first step is electronic photoexcitation of the solid. Photocarriers play main role in all three phenomena involving in self-cleaning properties of materials. However, the current situation in this research field, accompanying the high practical demand for self-cleaning nanocoatings based on photoactive materials, is characterized by a lack of a generally accepted hypotheses for understanding mechanisms of the process being under consideration.

The present study is devoted to the comparative study of self-cleaning properties of TiO_2, ZnO-based photoactive materials. The aim is to understand principles of creating surfaces with effective self-cleaning properties. The choice of semiconductor materials for the heterostructure construction came from the electronic structure and difference in photoinduced hydrophilic behavior. It implies the charge separation during the photoexcitation of created heterostructured materials.

The complex study of photocatalytic activity, photoinduced hydrophilicity and antibacterial acting under light with different spectral composition is planned for composite coatings and powdered samples based on titanium dioxide and zinc oxide. Experimental data were obtained by variety of approaches and techniques.

It was found that photoinduced surface hydrophilicity of TiO_2 and ZnO thin films can be dramatically changed by creation of heterostructures. Testing of the photocatalytic activity of dispersed ZnO and TiO_2 oxides and heterostructured coatings, as well as coatings based on the photoactive composites with titanium and zinc oxides, in the gas (photooxidation of acetaldehyde) and liquid (photocatalytic decomposition of phenol, decolorization of methylene blue) phases. Testing of antibacterial activity against E. coli strain of ZnO, TiO_2 and their composites.

All these data help to answer the question, what type of photocarrier or their ratio alteration is responsible for different photoprocesses providing self-cleaning properties of individual materials, TiO_2 and ZnO, and their heterostructures.

Audience Take Away:

- Novel scientific approach to the design of effective self-cleaning coatings.
- Highlights on the interconnection of photocatalytic activity, photoinduced bactericidal acting and photoinduced hydrophilicity of the TiO_2, ZnO-based photoactive materials.
- Our research could be useful to other faculty to expand their research or teaching in material science.
- Our study provides a practical solution to a problem of self-cleaning coating creation that makes the researcher's job more efficient.

Biography

Aida Rudakova received her PhD in physical chemistry in 1999 at University of Tomsk, Russia. Since 2014 she is a Senior Researcher and a Head of the Division ”Synthesis of Photoactive Materials” at the Laboratory of Photoactive Nanocomposite Materials at the Saint-Petersburg State University. Areas of her professional interests are heterogeneous catalysis and photocatalysis, photoinduced hydrophilicity/hydrophobicity, synthesis and characterization of photoactive materials. 25 scientific publications, 4 patents, and more than 40 oral and poster presentations on the international conferences present scientific work of Dr. Aida Rudakova.

CONTENTS

Acetylation of aldehydes catalyzed by acid phosphonium organoclays

Luboš Jankovič, Ph.D.
IIC Slovak Academy of Sciences, Slovakia

The protection of aromatic aldehydes with acetic anhydride was investigated in the catalytic presence of acid activated four alkylphosphonium exchanged montmorillonites (Px-MMT). The acid sites of all catalysts were investigated by infrared spectroscopy and thermal analysis using pyridine as a molecular probe. The yield of reaction is roughly related to the strength of acid sites and depends also on the substitution on the benzene ring of the aldehydes. The order of activity of selected organocation-exchanged forms was P16>P28>P32~P40 which correlates well with the size of these cations and resulting acidity. P32-MMT is revealed to be an effective catalyst for protection of aromatic aldehydes with Ac_2O and produces almost solely 1, 1-diacetates.

Audience Take Away:

- Participants may be involved into collaboration with our institute or I can explain them in details how to effectively prepare a new kind of solid catalysts based on alkylphosphonium organoclays.
- Participants could use these scientific results to expand their research or teaching.
- Data present here may help to develop completely new kind of reusable catalysts suitable for wide span application in academic and in industry.

Biography

Luboš Jankovič mainly focuses on preparation of various catalysts by chemical modification of inorganic nanoclays and characterization of these organo-inorgano hybrid materials by various techniques XRD, IR, NMR, SEM, TG, etc

Mechanism of water oxidation and reversible proton dissociation on aquo-bridge between Ru(II) centres on dinuclear complexes

Shunsuke Watabe*, Taisei Sato, Kenji Saito, Tatsuto Yui, Masayuki Yagi
Niigata University, Japan

The ruthenium(II) complexes with polypyridyl ligands have been extensively studied due to the unique photochemical and photophysical properties and known to work as water oxidation catalyst. We have already reported dinuclear ruthenium(II) complex chelated by 5-phenyl-2,8-di(2-pyridyl)-1,9,10-anthyridine, and it works as an efficient catalyst for water oxidation. Herein we report another type of dinuclear ruthenium(II) complex chelated by 2,7-bis(2-pyridyl)-1,8-diazaanthracene with rare bridge structure of μ-aquo, μ–hydroxo and μ-oxo. The activity of electrocatalytic water oxidation is compared with those having the anthyridine backbone structure.

Audience Take Away:

- Water oxidation catalysis, complex chemistry, intermolecular interaction

Biography

Shunsuke Watabe received his master's degree from Niigata University in 2017. He went on to the Ph.D course of Graduate School of Science and Technology in Niigata University in the same year.

Synthesis and photocatalytic activity of $CoFe_2O_4$/Reduced graphene oxide nanocomposites

Kun-Yauh Shih*, Yi-Shu Wang, Shou-Shiun Yang
Department of Applied Chemistry, National Pingtung University, Pingtung, Taiwan

To eliminate organic pollutants, the Photo-Fenton reaction is an advanced approach. Graphite oxide was prepared through modified Hummers method in this study. By microwave assisted method, cobalt ferrite/reduced graphene oxide composites were synthesized. The chemical structure and properties of composites were characterized by Raman spectroscopy, then the prepared $CoFe_2O_4$/RGO composites were employed into experiment of degradation. The Raman spectroscopy demonstrated the peaks in low-frequency (200-700cm^{-1}) were conformed to scattering modes of $CoFe_2O_4$, the Raman intensities ID/IG of composite increased obviously as the synthesis time on microwave increased may attributed to the forming the smaller sp^2 domains during the reduction process. Moreover, different catalyst composites were introduced into photo degradation experiment under UV-light, the results showed the catalytic activity of $CoFe_2O_4$ was enhanced greatly by introduction of reduced graphene oxide. Meanwhile, the composite with microwave time 200 second found out to show the greatest degradation activity, which maintained 90% of performance ability for five times recycling test.

Biography

Kun-Yauh Shih received his BS and PhD degrees in Chemistry from Tunghai University in 1986 and National Tsing Hua University in 1992, respectively. He has been Professor in Department of Applied Chemistry at National Pingtung University, Taiwan, since 2000. His current research interests are in the area of nanomaterials and energy technology with emphasis on the development of functional materials for photocatalysis, phosphor and electrode material applications.

CONTENTS

Catalytic performance of galloaluminosilicates in aromatization of lower alkanes: A comparative study with Ga/HZSM-5

Mohammad Naseem Akhtar, Ph.D.
Center of Research Excellence in Petroleum Refining & Petrochemicals, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia

A series of gallium-containing HZSM-5 zeolites with different Ga contents (Ga/(Al+Ga) = 0.1–0.6) were prepared by hydrothermal in situ synthesis and post synthesis. Their catalytic performance were compared in the aromatization of propane, butane and propane/butane mixture (1:1 molar). Galloaluminosilicate obtained via hydrothermal in situ synthesis exhibited high fraction of acidic framework Ga^{3+} with few dispersed extracrystalline Ga_2O_3. Ga/HZSM-5 obtained by post synthesis showed the presence of extracrystalline Ga_2O_3 and/or extra framework gallyl ions. The aromatization performance of Ga-containing HZSM-5 followed the following sequence; galloaluminosilicate > Ga/HZSM-5 (ion-exchange) > Ga/HZSM-5 (impregnation) >> HZSM-5. Optimum aromatization performance over galloaluminosilicate was achieved with Ga/(Al+Ga) ratio of 0.3. Propane conversion reached 50.9 wt% over galloaluminosilicate with Ga/(Al+Ga) of 0.3, as compared to 31.8 and 40.7 wt% for the corresponding Ga/HZSM-5 obtained by impregnation and ion exchange, respectively, at gas hourly space velocity of 1,600 h-1, and 540 ˚C. Comparison of aromatic selectivity at the same conversion level (~10.0 wt%) revealed that galloaluminosilicate is more selective than Ga/HZSM-5. The superior performance of galloaluminosilicate was attributed to the presence of highly dispersed-reducible extra-framework Ga_2O_3 (Lewis-dehydrogenating sites) formed by degalliation in close proximity to zeolitic Bronsted sites. Thus, hydrothermal in situ approach can thus be considered as an effective method for improving the aromatization performance of HZSM-5.

Audience Take Away:

- Audience will be able to apply the concept of aromatization of alkane
- It will help them in designing novel catalysts for such type of applications in the area of petrochemicals.

Biography

Muhammad Naseem Akhtar is a Research Scientist-I/Associate Professor at the Center for Refining and Petrochemicals of the Research Institute, King Fahd University of Petroleum and Minerals (KFUPM), Dhahran, Saudi Arabia. He received his Ph.D. degree in Chemistry in 1996 from KFUPM, Dhahran, Saudi Arabia, and his M.Phil. and M.Sc. degrees in Chemistry from Quaid-E-Azam University, Islamabad, Pakistan in 1990 and 1987, respectively. He is a member of American Chemical Society, Saudi Arabian International Chemical Sciences Chapter of the American Chemical Society, and Saudi Arabian Section of American Institute of Chemical Engineers.

Akhtar has been active in research for almost two decades. His contributions in the field of petrochemicals are of great significance which addresses the developing technologies for polyolefin catalysis and conversion of low-value petroleum derived feedstocks into high-value petrochemicals products. Akhtar has been actively involved in several projects related to the petrochemicals for local and international clients. Akhtar has published several patents and international refereed journal papers in reputable journals and has participated in national/international conference in the area of petrochemicals, catalysis, and polyolefin. His research work has been widely cited in scientific literature and technical reports.

Size control of Ruthenium nanoparticles in Ruthenium/Carbon composites derived from metal-organic frameworks

Seoyoon Shin, Moo Whan Shin*, Ph.D.
School of Integrated Technology, Yonsei University, Republic of Korea

In order to utilize catalytic activities efficiently, while using minimum amount of catalysts, various synthetic methods have been attempted by deposition of catalytic nanoparticles onto a porous or/and conductive support. In the case of platinum, which is the most commonly used electrocatalyst, platinum is deposited by wet chemical method, vacuum deposition, or atomic layer. However, these synthetic methods have obstacles regarding effective dispersion and utilization of Pt catalyst. In addition, heterogeneous particle size and broad size distribution of Pt catalyst can be another obstacle exhibiting efficient catalytic properties. These days, many efforts have been implemented as a way to create composites materials by incorporating metal or metal oxide nanoparticles into various host materials. Among these candidates, carbonaceous materials using metal-organic frameworks (MOFs) as precursors have already enormous attentions. In this study, we report a successful synthesis of ruthenium/carbon composites via simple carbonization process of Ru-MOF under inert atmosphere. For the investigation of the effects of temperature on the microstructural development, Ru-MOF samples have been carbonized at different temperatures from 300, 500, 700, and 900ºC in a horizontal quart tube furnace. The microstucture of the composites was observed by field-emission scanning electron microscopy (FESEM) and high-resolution transmission electron microscopy (HRTEM). It was founded that the Ru-MOF have the cubic morphology covered with particles which are considered to be ruthenium nanoparticles that have not been synthesized in the form of Ru-MOF. As the carbonization temperature increases, the size of the ruthenium particles increases with the sizes of 2-3 nm, 3-4 nm and 5-7 nm for the carbonization temperatures of 500, 700, and 900ºC, respectively and the shape becomes uneven with an agglomeration. The growth of the nanoparticles phenomenon is explained by a particle migration and coalescence (PMC) or Ostwald ripening mechanism. Structural and electrochemical characterizations reveal that carbonization temperature plays a critical role for the determination of the degree of graphitization and Ru particle size. This study suggests a simple and effective way to control the size of the metal obtained by carbonization of MOF, which provides a perspective in many fields of chemical or energy applications of Ru-MOF and others.

Audience Take Away:

- Application of Ru-MOF synthesis method to fabrication of other MOFs and characterization process.
- Perspectives on microstructure-properties relationship is always important in research. In this study, the microstructure development of MOFs and detailed process of MOF synthesis are co-related for the optimization of potential performance of MOF.

Biography

Moo Whan Shin is currently a Professor in the School of Integrated Technology at Yonsei University. He received Master and Ph.D in Materials Science and Engineering from the North Carolina State University, USA in 1988 and 1991, respectively. He holds 35 patents and published more than 250 papers at international journals and conferences on energy materials, semiconductor processing and devices. He was a President of Korea Society of Optoelectronics. He served Korean government as a member of Presidential Committee on Green Growth. His current research interests include development of nano structures for energy and application of solid state laser to the synthesis of novel electronic and electrochemical structures.

Activated carbons from used motor oil as catalyst support

Izabela Georgieva Genova*[1], Ph.D., T. Tsoncheva[1], S. Marinov[1], Ph.D., N. Petrov[1], Ph.D., N. Velinov[2] Ph.D., L. Gonsalvesh-Musakova[3], Ph.D., I. Spassova[4], Ph.D., D. Kovacheva[4], Ph.D.
[1]Institute of Organic Chemistry with Centre of Phytochemistry, BAS, Bulgaria
[2]Institute of Catalysis, BAS, Bulgaria
[3]Prof. Assen Zlatarov", University, Bulgaria
[4]Institute of General and Inorganic Chemistry, BAS, Bulgaria

Recently, the catalytic methanol decomposition process is considered as the simplest way for syngas production. The development of active and low-cost catalysts for methanol decomposition forced their usage in nanoscale by deposition on suitable, generally porous supports. Activated carbon (AC) can be used for this purpose due to its high surface area, porous structure, specific surface reactivity and possibility to be derived from renewable and waste materials, such as biomass and various organic residues. In our previous study we demonstrated that activated carbon from biomass wastes are appropriate catalyst supports for spinel ferrites. The effect of texture and surface characteristics of the activated carbon host matrix, prepared from different biomass precursors, such as grape seeds, peach and apricot stones, was study and compared with mesoporous silica type KIT-6. This study is aimed at the investigation of possibility to use activated carbon from used motor oil, as a host matrix for nanosized zinc ferrite nanoparticles. The attention was focused on the role of texture and surface characteristics of carbon support on the regulation of the state of active phase. For the purpose, series of AC with tunable characteristics, which were achieved by some specific post synthesis treatments and by using used motor oil as a precursor and various wastes additives such as coal tar pitch and polymers, were used as host matrix for zinc ferrite nanoparticles. A simple wetness impregnation technique ACs supports modification was applied. The catalytic behaviour of the obtained metal oxide composites was tested in methanol decomposition in view of its potential application as intelligent carrier of hydrogen. The effect of carbon support on the formation and state of zinc ferrite phase will be followed in detail.

Biography

Izabela Genova is an Assist. Prof. in Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Science, lab." Organic Reactions on Microporous Materials". The results of her work are formed in 27 publications, 23 of which in scientific journals with an impact factor. She has participated in 41 international scientific conferences with oral and poster presentations.

Synthesis of Rice-Ear-Shaped Cu dendrites by Galvanic displacement

Jong-Hyun Lee*, Ph.D., Jun Ho Hwang
Department of Materials Science and Engineering, Seoul National University of Science and Technology, Republic of Korea

Rice-ear-shaped Cu dendritic particles were fabricated through fast galvanic displacement reactions for 3–5 min under ambient conditions by adding Zn particles into an aqueous electrolyte without chlorine ions. The Cu dendritic particles had a small average size (4.44 μm) and short, multiple branches that seemed to be aggregates of nanoparticles were formed on backbone stems, exhibiting large surface area. The Cu dendrites could be protected against oxidation during drying by post-treatment. While the dendrite stem was a polycrystal grown only on the (111) plane, the branches consisted of three planes (111), (200), and (220), indicating that they were formed by random attachment of nanoparticles and aggregates. A possible low-temperature and high-speed synthesis mechanism was discussed with results of time-dependent SEM investigations as well as TEM studies regarding the crystal structure of the dendrite. This novel technique to synthesize the modified dendrites is extremely simple and suitable for mass production.

In this study, we have synthesized Cu dendrite powders using galvanic displacement of Zn powder. The Zn powder disappears, allowing easy collection of the Cu dendrites. The morphology and time-dependent evolution of the dendrites are analyzed in detail. We believe that our study makes a significant contribution to the literature because the updated processing method, the mechanisms of which are detailed in the study, provides a fast synthesis with a high yield, and is suitable for mass production. Further, we believe that this paper will be of interest to the readership of your journal because it elucidates the mechanisms involved during synthesis and processing of Cu dendrites.

Biography

From 2001 to 2005, Jong-Hyun Lee was with ETRI, Daejeon, Korea, where he was involved in developing optoelectronic packages. In 2005, he was with the Memory Device Division, Samsung Electronics Corporation, Onyang, Korea. From 2006 to 2008, he was a senior researcher of Korea Institute of Industrial Technology (KITECH), Incheon, Korea, where he worked on electronic packaging materials and processes. Since 2008, he has been working as an assistant professor at the Department of Materials Science and Engineering, Seoul National University of Science and Technology, Seoul, Korea.

CONTENTS

Catalytic H_2O_2 production via water oxidation by a dinuclear ruthenium complex

Yuuki Tanahashi*, Keitaro Kaneko, Kosuke Takahashi, Kenji Saito, Tatsuto Yui, Masayuki Yagi
Niigata University, Japan

Artificial photosynthesis has attracted attention as one of solutions to energy and environmental problems. A catalyst for water splitting into hydrogen and oxygen in artificial photosynthesis is important to be developed. In this context, much effort has been paid for development of molecular catalysts for water oxidation. There are only a few reports on a catalyst for hydrogen peroxide production via water oxidization. Herein we report catalytic hydrogen peroxide production via water oxidization by a dinuclear ruthenium complex. We found that for this dinuclear ruthenium (II) complex, an OOH bridging is formed oxidatively from OH and H_2O ligands in basic conditions. The activity and mechanism of catalytic hydro peroxide evolution in homogeneous solution will be discussed.

Biography

He received his master's degree from Niigata University in 2018. He went on to the Ph.D course of Graduate School of Science and Technology in Niigata University in the same year.

All-atom molecular dynamics of a ternary mixud of phospholipids

Nahuel Armando Moreno[1], Gloria Arlette Mendez[2], Efrain Urrutia Bañuelos[1]*
[1]Departamento de Investigación en Física. Universidad de Sonora. Blvd Luis Encinas y Rosales SN, Centro, 83000 Hermosillo, Son. Mexico
[2]Cátedra Conacyt-Facultad de medicina, Universidad Autónoma de San Luis Potosí, Avenida Venustiano Carranza 2405, Los Filtros, 78210 San Luis Potosí, S.L.P. Mexico

Since the formalization of the lipid raft concept in 1997, there has been a lot of controversy about the existence of this elusive raft. This is because seeing is believing and we can not elucidate it for direct methods due to its spatial and time scale. However, some indirect methods for the detection of this peculiar packaging, have shown that this process indeed exists. Also, the physicochemical properties responsible for the lateral compartmentalization and the molecular mechanisms involved in this process remain unclear until today. One advantage that could be of great help is the superior calculus capacity of a computer with which you could model a complex system. With this in mind we try to understand the physical inside of this phenomenon, helped with molecular dynamics simulation. In our analysis we want to make as many inferences as we can with the data available from the simulation. In this work we presente results of simulation of 400 moleculars palmitoyloleoylphosphatidylcholine (POPC), 342 of palmitoylsphingomyelin (PSM) and 400 of cholesterol, obtaned with GROMACS. To trying to understand their molecular structure we calculated the radial distribution function, the density profile and the order parameters. We also analyze the coefficient of diffusion and the change in time of the area per lipid.

Audience Take Away:

- The method we use to simulate the interaction of phospholides in water.
- How to reproduce a phenomenon in wich the cholesterol play the role of a classifier capable of packaging phospholipids, in particular the ones with saturated tails.
- Results of the Structural and lateral diffusion (on the surface of the membrane) of the lipid rafts.

Biography

Efrain Urrutia Bañuelos was born in June 1, 1959 in Queretaro Qro. Mex. Study the Bachelor in Physics and the Doctorate in Physical Sciences at the University of Sonora in Mex. I work at the University of Sonora in the Physics Research Department. My position is Research Professor. My research is in materials such as colloids, liquid metals and supercooled, through computer simulation.

A novel, low cost material for automotive catalysis

Alexander Dennis James*, Prof. Hu Li, Prof. John M. C. Plane
School of Chemistry, University of Leeds, UK

Catalytic processing of vehicle exhaust emissions to reduce their impacts on air quality currently requires large quantities of expensive Platinum Group Metals (PGMs). Whilst technologies for oxidation of CO are relatively mature, new materials capable of catalysing the reduction of NO_x are needed in order to meet emissions targets. Here we present a novel, low cost material (LowCat) capable of catalysing CO oxidation and NO_x reduction simultaneously. The mechanism of action of the catalyst is investigated both computationally and experimentally to inform its real world use. The LowCat material binds O_2, which can then oxidise two equivalents of CO, NO can also be oxidised by this surface O_2, a temperature dependent process observed here above 175°C, yielding NO_2 in the gas phase and an isolated O bound to the surface. NH_3 can bind to a neighbouring site, yielding NH_2 and OH radicals on the surface. NO can react with the NH_2 to give N_2 and H_2O, whilst a further NH_3 inserts into the bond between the OH and the surface. Reaction of a further NO, either with this bound complex or an NH_2 radical after emission of H_2O, produces further H_2O and N_2. The lone surface bound O, which is crucial to the further sequence of reactions leading to NO reduction, is also readily produced from surface reduction of NO_2 to NO. This route for producing surface O from NO_2 is active and allows reduction of NO_x even at room temperature. This mechanism is in agreement with previous results on similar catalyst surfaces, but with catalytic rates sufficient to produce reduction of NO_x in real world engines. Such an efficient, affordable catalyst capable of simultaneously oxidising CO and reducing NO_x even from cold start engines could have significant impacts on human health.

Audience Take Away:

- A low cost, effective alternative exists to commercial automotive catalysts.
- The mechanism of action of this catalyst has been explained by a combination of computational and experimental techniques, which agree remarkably well.
- The resulting thorough understanding of the mechanism of action allows a quantification of the kinetics of NO_x reduction.
- The measured kinetics can then be used to show that LowCat is competitive with industry standard technologies.

Biography

Alexander D. James received a Masters in Chemistry with Environmental and Sustainable Chemistry from the University of Edinburgh in 2012. He then received a Ph.D. for his work on the impacts of meteoric material on planetary atmospheres from the University of Leeds, in 2017. The focus of this thesis, supervised by John Plane, was heterogeneous catalysis of atmospheric processes including uptake, reaction and nucleation of crystallisation. Alexander then secured an ERC Proof of Concept grant to work on exhaust catalysis in collaboration with the School of Chemical and Process Engineering, University of Leeds, which forms the basis of this presentation.

Pd/DNA as highly active and recyclable catalyst of Suzuki-Miyaura coupling and aminocarbonylation. XPS investigation

Wlodzimierz Tylus*[1], Ph.D., Mehmet Mart[2], Anna Trzeciak[2]
[1]Wroclaw University of Science and Technology, Poland
[2]University of Wroclaw, Poland

Palladium is common known as best catalyst in the Suzuki–Miyaura and carbonylative coupling reactions due to its very high efficiency. Despite this, searching for new palladium catalysts is still a challenge. Not only complexes but also palladium nanoparticles (Pd NPs) should be taken into account, due to their unique physical properties differ from those of bulk metals and metal complexes. The successful application of Pd NPs requires their good stabilization against agglomeration.

DNA is a biopolymer with many unique features. It has been proved suitable as a template for metal and metal oxide nanoparticles, only scarcely employed in catalysis. DNA-supported Pd NPs were prepared out of cheap natural DNA at mild conditions in $EtOH/H_2O$ solution, without additional reducing agent. An effect of the palladium precursor and its dosage, on the various palladium nanoparticles sizes and morphology of Pd/DNA was observed (XPS, TEM, XRD, FTIR, SEM). The chemical shift in binding energy of XPS Pd 3d increased with the increase in the Pd(0) content indicated the interaction (immobilization) of Pd NPs with the DNA surface.

The Pd/DNA catalysts prepared from $Pd(OAc)_2$ exhibited various activities; however, the best result was noted for Pd/DNA containing mainly Pd(II) and only a small amount of Pd(0). The calculated content of Pd(0) present in the catalysts prepared at RT (C1) and at 80° C (C2) was 20% and 45%, respectively. It was proved that the most catalytically active Pd(0) was formed under catalytic reaction conditions. For both, C_1 and C_2 catalysts, the proportion of metallic palladium increased to above 80%.

The catalyst was recovered by simple phase separation and then reused in seven consecutive cycles with a high activity. For the first time, Pd/DNA was applied with very good results in the carbonylative coupling of iodobenzene, leading to amides, benzoic acid, or benzophenone depending on the kind of nucleophile used. Aminocarbonylation of iodobenzene with n-hexylamine was performed with excellent selectivity using $Mo(CO)_6$ as a CO source, while a mixture of products was formed with gaseous CO. The recovered Pd/DNA catalyst was used in the next four runs with high activity.

Audience Take Away:

- The Audience will be able to learn and discuss the methodology of interpreting complex XPS spectra
- Applying QUASES-Tougaard Software for modelling of Surface Nano-structures of catalysts
- Acquainted with the new method for the synthesis of nanoparticles of palladium and DNA (salmon fish sperm)

Biography

Wlodzimierz Tylus studied physics at the Wrocław University of Science and Technology . He received his master's degree of physics in 1981. His PhD degree received from Institute of Inorganic Technology and Mineral Fertilizers in 1988. He currently works as Associate Professor (Hab.) at Department of Advanced Material Technologies, Faculty of Chemistry, Wrocław University of Science and Technology.

His research interests mainly focus on the application of the XPS technique combined with other complementary techniques (SEM, TEM, XRD, FTIR,…) in the investigation of processes taking place on the surface of solids, i.e. homo- and heterogeneous catalysis, the plasma modification of polymer materials, corrosion, the ageing of materials and the formation of protective coatings. He is co-author of about 70 publication (h-index=22 and over 1300 citation), 5 patents and one book: "X-ray photoelectron spectroscopy in materials research. Selected examples of application."

Terminology spectrum analysis of natural-language chemical documents: Application on catalysis

Andrey O. Kuzmin*[1,2], Boris L. Alperin[1], Dr. Ludmila Yu. Ilina[1], Dr. Vladimir D. Gusev[3], Dr. Natalia V. Salomatina[3], Prof. Valentin N. Parmon[1,2]
[1]Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia, pr. Lavrentieva 5, 630090
[2]Novosibirsk State University, Novosibirsk, Russia, Pirogova 2, 630090
[3]Sobolev Institute of Mathematics SB RAS, Novosibirsk, Russia, acad. Koptyug avenue 4, 630090

This study is devoted to a methodology for automatic extraction of a complete set of ‘term-like phrases’ and to create a terminology spectrum from a collection of natural language PDF documents in the field of chemistry and catalysis. The ‘term-like phrase’ is one or more consecutive words and/or alphanumeric string combinations with unchanged spelling which convey specific scientific meaning. A terminology spectrum for a natural language document is an indexed list of tagged entities including: recognized general scientific concepts, terms linked to existing thesauri, names of chemical substances/reactions and term-like phrases. The retrieval routine is based on n-gram textual analysis with a sequential execution of various ‘accept and reject’ rules with taking into account the morphological and structural information.

It is suggested to use such terminology spectra to perform various types of textual analysis across document collections. Terminology spectrum may be successfully employed for text information retrieval and for reference database development. For example, it may be used to develop thesauri, to analyze research trends in subject fields of research by registering changes in terminology, to derive inference rules in order to understand particular text content, to look for the similarity between documents by comparing their terminology spectrum within an appropriate vector space, to develop methods to automatically map document to a reference database field.

For instance, if a set of documents contains texts from different time periods, the analysis of textual and absolute frequencies of occurrence will allow to follow up the “life cycle” of each term-like phrase on the quantitative level (term usage increasing, decreasing and so on). That gives unique capability to find out research trends and new concepts in a subject field by registering changes in terminology usage in the most rapidly developing areas of research. Moreover, similar dynamic of change over time for different terms often indicates the existence of an associative linkage between them (e.g. between new process and developed catalyst or methodology). Indicator words or phrases such as “for the first time”, “unique”, “distinctive feature” and so on may be also used in addition to detect in texts, for example, the new recipes or catalyst composition for the explored process.

The assessment of the retrieval process, expressed quantitatively with a precision (P), recall (R) and F1-measure, is made with using the text abstracts belonging to several catalytic conference events.

Audience Take Away:

- New ways to make scientific thesauri.
- Find out new research trends.
- Help to make new decisions on future research.

Biography

Andrey Kuzmin is senior researcher in Boreskov Institute of Catalysis SB RAS (BIC) and senior teacher in Novosibirsk State University (NSU). He graduated from NSU and received PhD degree in BIC. Fields of interests – intensification of chemical processes, data analysis. His last researches are connected with intensification of multiphase processes and chemical data acquisition from text collections.

Application of solution plasma method to preparation of Ag loaded Ga_2O_3 photocatalysts

Tomoko Yoshida[1]*, Ph.D., Naoto Yamamoto[2], Muneaki Yamamoto[1], Ph.D., Shinya Yagi[2], Ph.D.
[1]Osaka City University, Japan
[2]Nagoya University, Japan

Reduction of carbon dioxide (CO_2) with photocatalysts, an artificial photosynthesis, has been widely studied from the viewpoints of contribution to the energy, environmental and carbon resource issues. The photocatalytic reduction of CO_2 with water is one of the most challenging catalytic reactions, because the reduction ability of water is much lower as compared to other reduction reagents such as hydrogen (H_2). Recently, we found that the photocatalytic reduction of CO_2 with water proceeded over a bare Ga_2O_3 and the activity increased by loading Ag nanoparticles on Ga_2O_3 (Ag/Ga_2O_3). The photocatalytic activity is likely to correlate with the chemical states and/or the size of the Ag nanoparticles which depend on the preparing method of the photocatalysts.

In this study, we prepared Ag/Ga_2O_3 photocatalysts by using solution plasma method (SPM). The SPM is a new preparing method of metal nanoparticles without any dispersants in an aqueous solution with electrolytes. The Ag nanoparticles were synthesized by glow discharge between Ag rods in an aqueous solution. The synthesized Ag NPs were loaded on gallium oxide (Ga_2O_3) photocatalyst by filtering the solution with Ga_2O_3 powder, and the photocatalytic activities of the obtained Ag/Ga_2O_3 samples were evaluated.

Although the photocatalytic reduction of CO_2 with water proceeded over all the Ag/Ga_2O_3 photocatalysts to produce CO, the CO production rates decreased with the reaction time. Measurements of DR UV-vis spectra and TEM images revealed that a part of the Ag NPs migrated and aggregated on the photocatalyst surface to become larger particles during the photocatalytic reaction, which would be related to the decrease of the photocatalytic activity. It was also found that the photoirradiation treatment on the prepared Ag/Ga_2O_3 sample before the use for the photocatalytic reaction improves the photocatalytic performance.

Audience Take Away:

- The audience will be introduced to a solution plasma method (SPM), a new useful and simple preparation method of metal nanoparticle cocatalysts. The SPM has the advantage of fabricating size-controlled metal nanoparticles by the glow discharge between metal rods with electrolytes in an aqueous solution without any dispersants.

Biography

Tomoko Yoshida is professor of physical chemistry at Osaka City University Japan. In 1996, she completed Doctor's Course in Kyoto University and received her PhD in engineering. His research focuses on establishment of a new structural and electronic state analysis using synchrotron radiation spectroscopy and electron microscope to develop solid-state photocatalysts that promote artificial photosynthesis.

Depolymerisation of lignin over Ru-based heterogeneous catalysts

Verziu Marian Nicolae*[1], Ph.D., Alina Jurca[2], Ph.D., Aurore Richel[3], Ph.D., Jyri Pekka Mikkola[4], Ph.D.
[1]Institute of Organic Chemistry 'C. D. Nenitescu' of Romanian Academy, Romania
[2]University of Bucharest, Romania
[3]University of Liege– Gembloux Agro-BioTech, Romania
[4]Umeå University, Romania

Depolymerision of the lignin, extracted from Mischantus plant, was carried out both over mixed oxides such as $(NiRuMgAlO)_x$, $(NiRuAlO)_x$, $(NiAlO)_x$, $(NiMgAlO)_x$ derived from layered double hydroxides precursor and Ru supported on mesoporous alumina. The insertion of ruthenium in the structure of layered double hydroxides (Ni-(Mg)-Al) led to an increase of the surface area (highlighted by nitrogen physisorption) but also acidity (evidenced by NH_3-TPD) (Table 1 and Figure 1). Moreover the introduction of Ru by substitution did not influence the parent structure.

Tabel 1. Textural characteristics of the investigated catalysts

Catalyst	**Surface area (m^2/g)**	**Pore size (nm)**
$(RuNiMgAlO)_x$	126	4.6
$(NiMgAlO)_x$	102	5.3
$(RuNiAlO)_x$	171	4.9
$(NiAlO)_x$	166	7
Ru/Al_2O_3	226	8.6

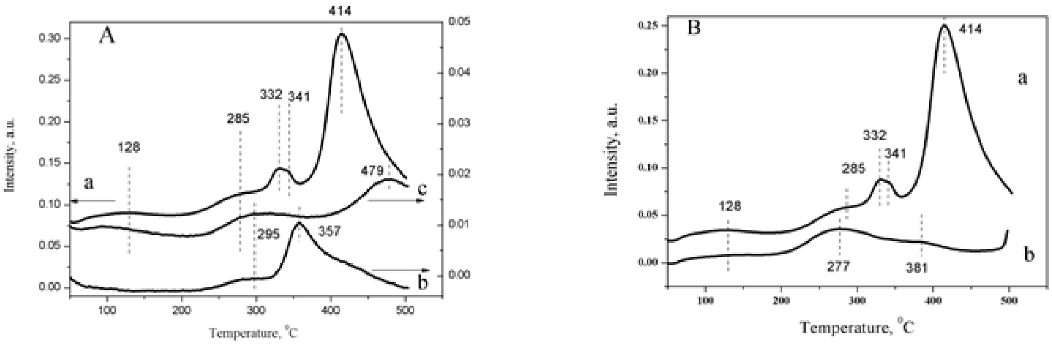


Figure 1. NH3-TPD profiles for : A: (a) $(RuNiAlO)_x$; (b) $(RuNiMgAlO)_x$; (c) Ru/Al2O3

B: (a) $(RuNiAlO)_x$; (b) $(NiAlO)_x$

If the XPS characterisation of these materials showed us the oxidation state of the ruthenium, the Ru-O-Ni bond formation was highlighted by Raman spectroscopy (Figure 2), thus the insertion of the Ru into mixed oxides structure led to a decrease of the bands intensities in the ranges 300-400 cm^{-1} and 900 to 1200 cm^{-1} ,characteristics of RuO_2 as bulk, due to due to dispersion of Ru in the (NiAlO)x network and Ru-O-Ni bond formation (Figure 2).

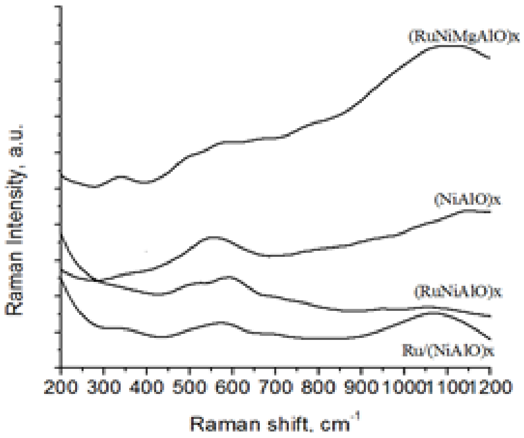
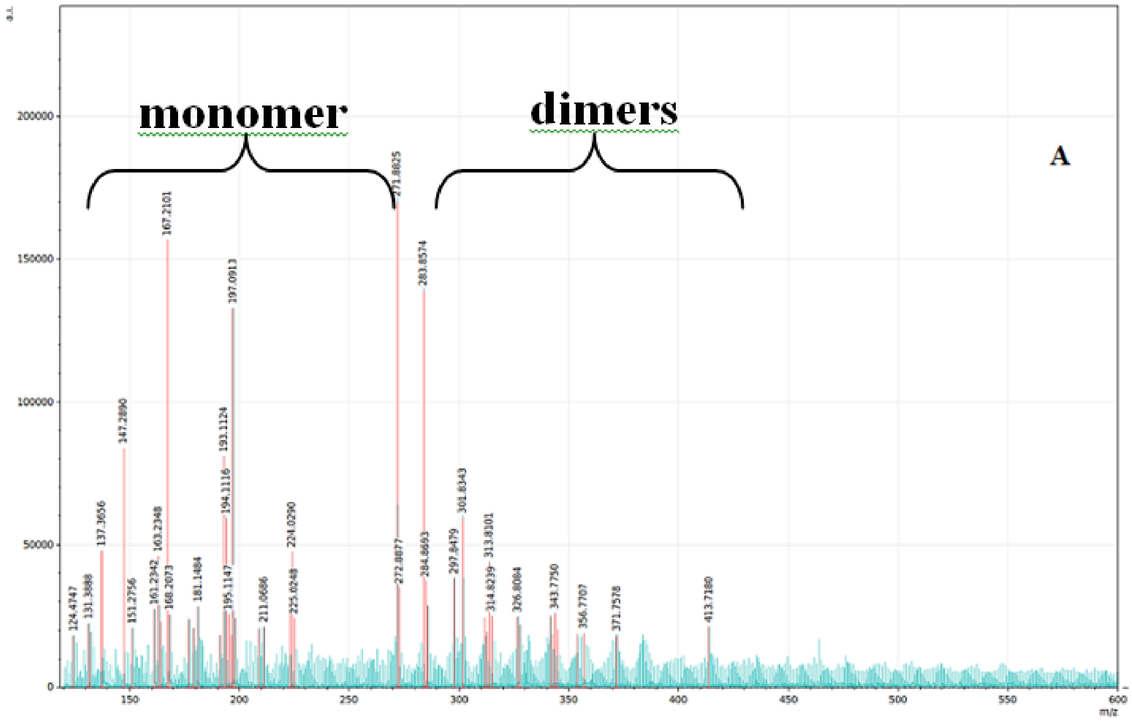


Figure 2. Raman spectra of $(RuNiAlO)_x$, $(NiAlO)_x$, $(RuNiMgAlO)_x$ and $Ru/(NiAlO)_x$

The hydrogenolysis of lignin was carried out under autoclave conditions and the reaction products were analysed both LDI-TOF-MS and HP-SEC techniques.

An interesting aspect was observed during the recycling test of the catalyst $(RuNiAlO)_x$. Although the ruthenium leaching was not detect upon the reaction, however after the third catalytic cycle a decrease of selectivity in dimers was noticed (Figure 3). This fact was due to sulfur poisoning whereas a sulfuric acid solution was used for the precipitation of the lignin extracted from Mishcantus plant. On the other hand the catalytic activity of this catalyst even after four catalytic cycles is due to the linkage between ruthenium and nickel which reduced the sulfur adsorption on the $(RuNiAlO)_x$ but the blocking of the active sites of ruthenium with sulfur led to a decrease of the dimers weight.



CONTENTS

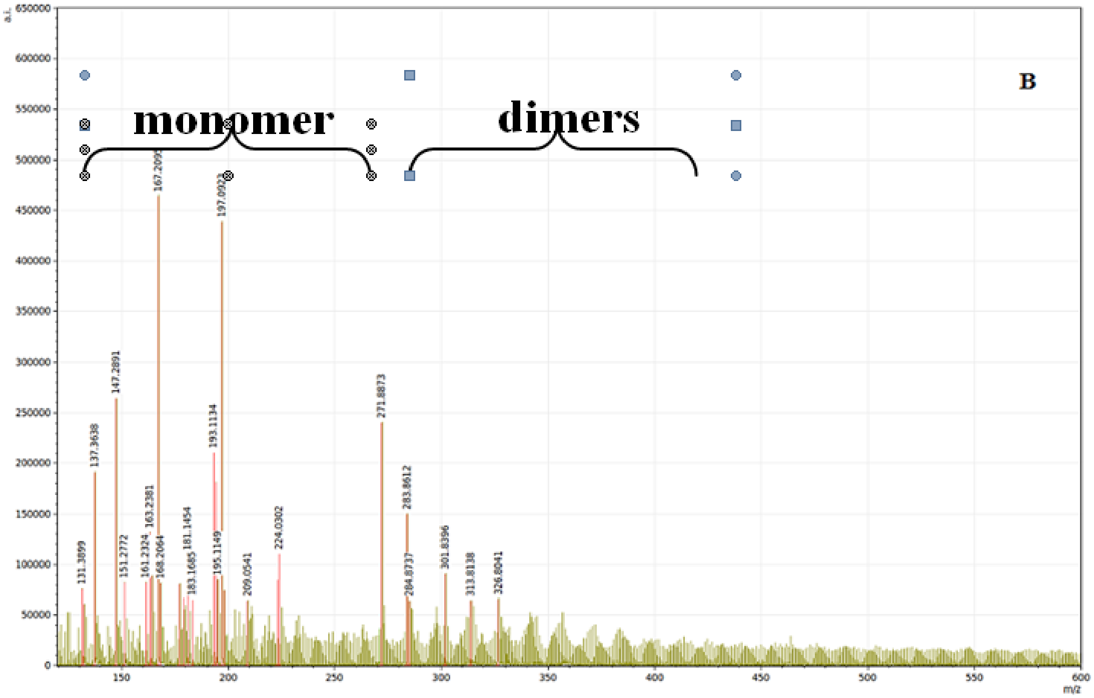


Figure 3. Reflector positive ion mode LDI-TOF-MS spectra of depolymerised lignin after third (A) and fourth (B) catalytic cycle over (RuNiAlO)x

Besides the presence of ruthenium, the amount of nickel influenced the catalytic performances in the hydrogenolysis of lignin, increasing slightly with the nickel content. Another factor which led to an increase of the lignin conversion was the acidity, thus the highest degree of lignin depolymerisation (conversion 89%) was carried out over Ru supported on alumina led to but the bimetallic synergism (RuNiAlO)x led to the best selectivity in the dimers production.

Audience Take Away:

Taking into account that the hydrogenolysis, one of the most promising methods in the depolymerisation of lignin, leads, especially to monomers formation by the C-O-C bond cleavage from lignin structure, we showed in this study that depolymerisation of the lignin over Ru-based heterogeneous catalysts led to an increase of the selectivity in the dimers formations. We also showed that:

- Presence of ruthenium led to dimers as dominant products
- The interaction between ruthenium and nickel had an increase of the catalyst stability.

Biography

2016 - Present: Researcher, Centre of Organic Chemistry "C. D. Nenitzescu", Romanian Academy, Bucharest, Romania
2013: PostDOC, University of Bucharest, Romania
2010: PhD degree, University of Bucharest, Romania
Professional skills:
Research experience in different areas:
- **Heterogeneous catalysis:**
 - Catalysts preparation (nanomaterials, oxides, LDHs, organic-inorganic hybrid systems).
- **Catalytic processes:** transesterification of triglyceride under conventional and nonconventional conditions; depolymerisation of lignine, cellulose
- Physicochemical characterization of the solids surface: XRD, DR-UV-Vis, Raman, DRIFT, BET, TPD, TPR
- **Analytical chemistry:** analysis of organic compounds by gas-chromatography (GC-FID, GC-TCD), liquid chromatography (HPLC and UPLC), mass spectrometry (MS, GC-MS, GC-MS-IR).

Publications:
8 articles (6 as main author)

CONTENTS

Particle interactions during solar TiO_2 photocatalytic treatment of organic matter

Ayse Hazal Pekcan Cetin*, Didem Saglik, Burak Demirel, Miray Bekbolet
Bogazici University, Turkey

Metal oxide nanoparticles have been used in several systems as photocatalysts recently. Light initiated degradation of the organic compounds is one of the most important application of these photocatalytic systems. Photocatalytic degradation of organic compounds in waters and wastewaters has been widely studied for many decades. TiO_2 is the most widely used photocatalyst due to its decent photocatalytic properties, ease to production and low cost. Major disadvantage of TiO_2 photocatalyst is its bandgap energy (E_{bg}=3.2 eV, □≤390 nm) for solar light activation since only 5% of solar light is UV light that can produce equal energy to TiO_2 band gap energy. Therefore, effective solar light utilization can be achieved with modifications through doping and/or coupling with other semiconductors such as ZnO. As an organic compound, natural organic matter degradation by photocatalysis has awoken interest for treatment systems and studied extremely in the last decade. Recently, Bekbolet and co-workers has been working on photocatalytic degradation of natural organic matter under solar irradiation, aiming to improve photocatalytic degradation yield with second generation photocatalysts. Beside the treatment efficiency, interactions between organic matter and metal oxides during photochemical reactions has also importance to understand possible further environmental applications. Formation of aggregates, a particle comprising of strongly bound or fused particles, and/or agglomerates, a collection of weakly bound particles, changes the system dynamics, so investigation of these interactions is essential. Furthermore, introduction of these particles to natural waters brings the question of "behavior nanoparticles in aqueous medium" that deserves attention to be elucidated in terms of diverse reactivities leading to deterioration of water quality. Elucidation of the interactions between metal oxide nanoparticles and natural organic matter will be done by using TiO_2 P25 as model nanoparticle and Suwannee River natural organic matter as organic matter. Characteristics of the binary system prior to, during and under post treatment conditions will be examined by UV-vis and fluorescence spectroscopy and physico-chemical properties will be assessed by particle size and zeta potential analysis and sedimentation experiments. The major outcome of the project would be to bring novel information to the understanding of the complex colloidal system operating under light leading to degradation of organic matrix via photolytic and photocatalytic oxidation pathways.

Audience Take Away:

As preliminary experiments and baseline information:

- Determination of UV-vis and fluorescence spectroscopic properties of natural organic matter,
- Determination of physico-chemical properties of photocatalyst,

Understanding of the physico-chemical behavior of the reacting partners:

- Application of specific physico-chemical methods, i.e. particle size distribution, zeta potential and sedimentation experiments,
- Elucidation of the characteristics of the binary system prior to-, during and under post treatment conditions.
- Application of UV-vis spectroscopic methods and organic matter quantification methods.

Biography

Ayse Hazal Pekcan Cetin obtained her B.S. in Chemistry from the Chemistry Department of Istanbul University in 2012. She received her M.Sc. degree entitled as "Montmorillonite and modified montmorillonite supported ZnO catalysts" from the Chemistry Department of the Institute of Graduate Studies in Sciences and Engineering of Bogazici University in 2015. Currently, she is a Ph.D. candidate and Research Assistant at the Institute of Environmental Sciences of Bogazici University. Her research interests include preparation and activity testing of novel photocatalysts, water treatment by advanced oxidation processes i.e. homogeneous and heterogeneous systems, photolytic/photocatalytic removal of natural organic matter specifically humic substances and UV-vis and fluorescence spectroscopic characterization of organic matter.

CONTENTS

Highly efficient and stable catalysts based on bimetallic Au@Ag nanoparticles decorated clay-poly(glycidylmethacrylate)

Samia Mahouche-Chergui[1]*, Abdallah Oun[1,2], Maryem Orfi[1,2], Raja Ben Amar[2], Benjamin Carbonnier[1]
[1]Université Paris-Est, ICMPE (UMR7182), CNRS, UPEC, Thiais 94320, France
[2]Laboratoire des Sciences de Matériaux et Environnement, Université de Sfax, Faculté des Sciences de Sfax, BP 1171, 3000 Sfax, Tunisia.

Nanostructured chelatant nanocomposites are emerged as promising platforms for homogeneous immobilization and stabilization of (bi)metallic nanoparticles. In this contribution, we report the preparation, characterization and catalytic applications of a new type of hybrid nanocatalysts based on gold and gold@silver mono- and bimetallic nanoparticles on polymer grafted-clay. Montmorillonite (MMT) clay was successively surfacegrafted with 3-(trimethoxysilyl)propyl methacrylate (ϒ-MAPS) and poly(glycidyl methacrylate) (PGMA) chains. The polymerization was conducted under UV-irradiation to ensure the fastgrowth of PGMA. The epoxy groups of MMT@PGMA have been readily converted into carboxylic acid and amino groups using $H_2SO_4/KMnO_4$ and ethylene diamine, respectively.

Finally, Au and Au-Ag nanoparticles have been synthesized through the in situ and hydrideassisted reduction of gold or silver followed by gold ions immobilized on amino or acid carboxylic-functionalized PGMA@MMT, respectively. The hybrid nanocomposites have been characterized after each synthesis step using a combination of complementary methods (TGA, TEM, XRD, FT-IR, XPS) providing information about chemical composition, structure, and morphology of particular interest, the TEM results indicated that Au and Ag-Au NPs with a spherical shape and narrow size distribution were homogeneously and densely dispersed at the surface of chelatant nanocomposites. The so-designed Ag-Au nanoparticles decorated MMT@PGMA ternary nanocomposites have shown noticeably enhanced catalytic activity than the monometallic AuNPs in the chemical reduction of nitrophenol (p-NP) and pesticide (pemdimethalin, PDM) pollutants in the presence of sodium borohydride with high recyclability for consecutive 5 runs. The UV-monitoring of the reduction reactions indicated that pseudo-first-order kinetics associated with a rate constant of 2.10^{-2} s^{-1} and $2.8\ 10^{-2}$ s^{-1} towards p-NP $1.2\ 10^{-3}$ s^{-1} and $4.3\ 10^{-3}$ s^{-1} towards PDM using MMT@PGMA-NH2@Au and MT@PGMACOOH@Ag-Au, respectively

Further progress aims at enhancing the catalytic performances of Au NPs-PGMA-MMT nanocomposite catalyst for the treatment of contaminated waste water via a hybrid process combining heterogeneous catalysis and membrane separation.

Biography

Samia Mahouche-Chergui obtained her Master degree in Inorganic Chemistry at Paris Sud University in 2006, and then her PhD in Surface-Interface Chemistry at Paris Diderot-P7 University in 2009. She worked then as a Lecturer/Researcher (ATER) in the same research Group developing a combination of diazonium compounds and click chemistry for the preparation of carbon hybrid materials. After postdoctoral research with Pr. Y. Grohens at the Bretagne Sud University from 2010 to 2012, she joined the East Paris Institute of Chemistry and Materials Science at the University Paris-Est Créteil as an assistant professor. Her research is currently focused on the development of sp2 carbon and clay based-functional hybrid nanostructures for applications including nanofillers, electrochemical sensors, and heterogeneous nanocatalysts.

Photocatalytic self-cleaning WO_3-rGO composite thin films for PV glazing

Maria Covei*, Cristina Bogatu, Dana Perniu, Anca Duta, Ion Visa
Transilvania University of Brasov, Romania, Renewable Energy Systems and Recycling Center

Photocatalysis has been used not only in water and air treatment but also, increasingly, in various domains such architecture (self-cleaning glass, tiles, cement), sanitation (clean room wall paint) and the PV industry. The use of protective coatings for photovoltaic glazing represents a hot topic at EU level, as an alternative method to increase the electrical output. One challenge is to simultaneously meet the requirements for photocatalytic self-cleaning properties and the specific optical properties in the full solar spectral range: high transmittance (T%) - low reflectance (R%) in UV-Vis and low T% - high R% in IR (IR-shielding properties).

Following the optical and the self-cleaning pre-requisites, a novel, sol-gel composite using WO_3 and reduced graphene oxide (r-GO) was obtained. Tungsten precursors (WCl_6, $WOCl_4$ or H_2WO_4) along with r-GO (0 - 5% wt.) were dispersed in water-ethanol mixtures (ratios of 1:0, 0:1 and 1:1). Acetylacetone and SDS were used at concentrations higher and lower than the critical micelle concentration to control particle nucleation and growth. The sols were aged for 48 h, dried and annealed at 550°C. The synthesis parameters were correlated with the crystallinity, morphology, surface energy and optical properties of the powders. Stable dispersions were prepared using the powders with high $T_{UV\text{-}Vis}$ - low T_{IR} and chitosan, to be sprayed on glass and solar glass. The results show that homogeneous, transparent thin films can be obtained using dispersions at optimized pH and concentration; the number of spraying sequences and the deposition temperature (40 - 60°C) are the key parameters in controlling the optical and self-cleaning properties. Promising photocatalytic efficiency values in phenol removal under simulated solar radiation (85% Vis and 15% UV) were obtained for the composite thin films, with the rGO outlining that this supports the increased charge separation.

Audience Take Away:

- The presentation reports on a new coating material for PV glazing, that can be directly applied on in-field modules, to decrease their energy loss;
- The coating material is delivered as a dispersion of a WO_3-rGO composite that, deposited on solar glass, forms thin films with good optical and photocatalytic properties.
- The presentation supports a knowledge extent on the novel WO_3-rGO photocatalytic composite systems (compared to TiO_2-rGO) to be used as powder and as sprayed thin film for organic pollutants removal (phenol) from aqueous media;
- The results are of interest for the PV manufacturers in identifying novel, alternative coatings for PV glazing, suitable for increasing the amount of solar radiation incident on the photovoltaic material, thus increasing the amount of electricity that can be expected to be produced.

Biography

Maria Covei (b. 1988) is part of the Renewable Energy Systems and Recycling Center in the Transilvania University of Brasov, Romania. Her field of expertise is on semiconductor oxides and chalcogenide thin films obtained through chemical deposition methods such as spray pyrolysis deposition (SPD) and the sol-gel technique. Her study of zinc oxide, titanium oxide, tin and tungsten oxide was aimed towards optoelectronic applications, with a particular focus on photocatalysis and photovoltaics. Her recent work focuses on the study of different composite structures based on metal oxide matrixes and carbon-based derivatives with tailored optical and photocatalytic properties for application as self-cleaning coatings.

Advancements in the process and catalyst developments for Ethylene Oxide and Ethylene Glycol: Current and future prospects

Muhammad Imran Yaqub*, Ph.D., Turki Al-Smar, Ph.D.
SABIC, Saudi Arabia

SABIC is the world largest MEG producer in the petrochemical sector. Ethylene oxide (EO) is a simplest form of epoxides and due to its molecular structure, it acts as a versatile intermediate for a variety of chemicals such as; monoethylene glycol (MEG), di- and triethylene glycols, ethoxylates, ethanol amines, and glycol ethers. The growing demand of MEG owing to its downstream utilization in polyester industry has prompted the research of an efficient, cost effective, and environmentally benign EO production process.

Currently, most of the World's MEG is being produced through conventional route; however, there is an increasing trend to exploit new routes, and feed stocks such as coal, bio-based, and Shale gas. The production capacity of MEG is expected to increase to 36 million tons by 2024. The heavy dependence of MEG producers on ethylene and its scarcity in some parts of the world promoted the need of alternate feedstock. The technological (process and catalyst) as well as commercial aspects will be discussed along with the future growth of EO/EG business.

Audience Take Away:

- The audience will learn about commercially used Silver based Ethylene Oxide (EO) catalyst
- Growth in EO catalyst and role of catalyst support
- Technological developments in the field of EO/EG

Biography

Muhammad Imran was born in January 1979 and received his BS Chemical Engineering in 2002 from Punjab University Lahore. Till 2004, Imran worked as a Process Engineer at Packages Limited (a pulp, paper, & packaging company). He then moved on to complete his MS (2006) and PhD (2010) in Chemical Engineering from Korea Advanced Institute of Science & Technology (KAIST), South Korea. After his PhD, he served University Technology Malaysia and King Saud University as a faculty member before joining SABIC in 2013. To his credit, there are several publications in high impact journals along with international conference proceedings.

Highly active molecular catalyst of a dinuclear ruthenium (II) complex for water oxidation

Hiroki Sonokawa*, Takashi Minamisawa, Taisei Sato, Kenji Saito, Tatsuto Yui, Masayuki Yagi
Niigata University, Japan

Widespread attention has recently been paid to artificial photosynthesis to resolve problems of environment and energy storage because a clean fuel such carbohydrate and hydrogen can be directly produced from water by abundant solar light. There is great interest in development of highly active catalysts for water oxidation, since catalysts for water oxidation are essential in construction of artificial photosynthesis. Mononuclear and dinuclear ruthenium complexes have been extensively studied as catalysts for water oxidation. Herein we report unique synthesis of a new series of dinuclear ruthenium (II) complexes. The highly activity of catalysts for water oxidation by these derivatives in homogeneous solution will be discussed.

Audience Take Away:

- Artificial photosynthesis, water splitting, water oxidation catalysis

Biography

Hiroki Sonokawa graduated from Niigata University (Japan) in 2018 and went on to graduate school in Niigata University.

Zeolites synthesized from fly ash for adsorption of phenol from waste water

Borislav Zhivkov Barbov[1]*, Ph.D., Yuri Kalvachev[2], Ph.D.
[1]Institute of Mineralogy and Crystallography, Bulgarian Academy of Sciences, Bulgaria
[2]Institute of Catalysis, Bulgarian Academy of Sciences, Bulgaria

The thermal power plants, based on coals, are the main source of fly ash (FA). Depending on the type of source and the composition of the coal being burned, the components of the solid by-products could vary considerably, but all FA includes substantial amounts of silica (both amorphous and crystalline) and alumina, both of them being endemic ingredients in many coal-bearing rock strata. FA is a fine powder captured from flue gas streams by dust collecting systems prior to their release into the atmosphere FA is generally stored in landfills. The disposal of FA creates ecological risks because of the acidification and the infiltration of heavy metals and radioactive components into the soil. The production of zeolite from FA is result in a good ingredient of high value as additive to cement. An attempt to find a common solution for this environmental problem is reported in the present work.

It was successfully synthesized zeolite Analcime (ANA) from FA produced by combustion of coal in three termal power plants using a one-stage process - hydrothermal synthesis. Initial synthetic gels were obtained by preparing of mixture with ratio Sodium hydroxide/FA in the range of 2.0 to 1. By decreasing the amount of NaOH, crystallization of zeolites ANA, SOD, CAN and NaP begins. In order to obtain the mono-phase product zeolite Analcime, additional silica powder was added to the synthesis mixture. The obtained samples were characterized by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). The adsorption capacity towards phenol of synthesized ANA-type zeolite samples were investigated for the purification of phenol-contaminated water.

Audience Take Away:

- Methods of recovery the coal fly ash – the synthesis of zeolites is with the highest added value.
- A method for synthesis of a ANA-type zeolite structure from coal fly ash
- Influence of the morphology and the particle size of the obtained zeolite crystals on their adsorption properties
- Influence of crystallization time, temperature of synthesis and various NaOH / FA ratios used in the study.
- Investigation of adsorption capacity towards phenol of synthesized zeolite ANA in order to be used for purification of phenol-contaminated water.

Biography

Borislav Barbov is a young scientist who received his PhD in 2017 from Institute of Mineralogy and Crystallography "Acad. Ivan Kostov" – Bulgarian Academy of Sciences (Sofia, Bulgaria), Department of Crystallography and Material Science where he continues to work. His research interests are focused in the fields of synthesis of zeolites in the presence of seeds, synthesis of zeolites from coal fly ash and structure and application of zeolites. Now he is working on a research project on a topic: Synthesis of zeolites from coal fly ash for environmental applications.

Catalytic hydrothermal gasification of organic compound

Isao Hasegawa*, Junichi Hayashi
Kansai University, Japan

Nearly many studies on gasification of organic compounds under hydrothermal or supercritical water conditions have been performed. In this study, we conducted the catalytic hydrothermal gasification of diluted lactic acid. Several catalysts were used for comparison in catalytic activities. We chose activated carbon, silica alumina and Nickel on silica alumina and the prepared Nickel on activated carbon as catalysts. Nickel on activated carbon catalyst was prepared as follows: Nickel nitrate and the activated carbon were mixed physically and were carbonized in nitrogen flow at 873 K for 1 hour. In gasification experiment, 5 mL of 2 wt.% lactic acid aqueous solution and 0.1 g of solid catalyst were filled in a stainless-steal reactor. The reactor was plunged into an oil bath preheated to a temperature of 250 °C, then the reaction pressure increased rapidly up to the saturated vapor pressure at the temperature. After an elapse of the reaction time, the reactor was immediately soaked in a cool water bath. The total organic carbon in the aqueous solution was estimated using a TOC analyzer. Gasification conversion was calculated from TOC measurement on the basis of carbon in the solution. Conversion of reactant (lactic acid) was estimated from the concentration before and after the reaction. Gasification conversion reached 20% with activated carbon, only 10% without the catalyst. The changes in the soluble products distribution with passage of time were examined. The other organic compounds such as acetaldehyde were still existent after the reaction for 3 h. These compounds are judged to be inactive against the gasification.

Audience Take Away:

- Difference in the catalytic activities for hydrothermal gasification
- Degradation paths of lactic acid under hydrothermal condition

Biography

Isao Hasegawa was graduated from the School of Industrial Chemistry, Kyoto University in 1999. He received his PhD in 2007. At present, he is an Associate Professor at the Department of Chemical, Energy and Environmental Engineering of Kansai University and his research interests focus on the development of the new thermochemical conversion of biomass, pretreatment methods and pyrolysis kinetics.

CONTENTS

Composite materials based on active carbon from biomass residues and zinc oxide nanoparticles for water purification

Cristian Răducanu, Alexandra Mocanu*, Dr. Oana Pârvulescu, Dr. Aurel Diacon
University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Gh. Polizu, Sector 1, Bucharest, Romania, RO-011061

Recent research concerning heterogeneous catalytic support for chemical synthesis or the development of new chemical compounds is governed lately by two principles: nanoparticle scale materials and sustainable materials. Using biomass residues and processes like pyrolysis and thermal activation or calcinations, we were able, in respect with these principles, to develop new materials for photodegradation processes of organic compounds from wastewaters.

The conversion of biomass residues into value-added products is in line with European directives for environmental protection, which are imposing stringent rules on the implementation of non-polluting organic waste recovery processes. Recent studies involved the fructification of biomass residues into active carbon (CA) in order to obtain composite materials for photocatalytic degradation reactions of organic compounds from contaminated water.

Furthermore, the degradation of organic polluting agents can also be performed successfully in the presence of metal oxides such as ZnO, TiO_2, ZrO_2, etc, due to their photocatalytic properties, relatively low synthesis costs and non-toxic actions towards environment.

The properties of CA obtained from biomass and used for water purification depend on the nature of biomass, pyrolysis and activation conditions.

Thus, in the first step, our study involved three different types of biomass, such as: algal residues, cherry pits and bacterial cellulose which were pyrolyzed and further activated in different conditions in order to obtain CA (as shown in Table 1).

Biomass	Pyrolysis reaction (in CO2 flow)	Yield of carbon % (g/g)	Activation temperature (°C)	Activation time (hour)	Activation gas
Algal residues (after protein isolation and oil extraction)	650 °C	42	1	920 °C	steam/CO2 complex
Cherry pits	780 °C	24,54	1	1200 °C	steam/CO2 complex
Bacterial cellulose	750 °C	36	1	1100 °C	steam/CO2 complex

The recovery of ZnO NPs by sedimentation or filtration could be a difficult task due to the decresed size of the inorganic particles. Thus, the immobilization of such particles on different substrates is necessary in order to better recover and reuse the composite material for a new photodegradation cycle.

For this reason, the next step consisted in the direct generation of ZnO nanoparticles (ZnO NPs) on the surface of CA using both conventional and unconventional reactions (ultrasound-assisted process) to develop composite materials with higher efficiency in the photocatalytic process.

In our case, depending on the ZnO synthesis procedure, the medium size diameter of the inorganic nanoparticles varied from 5 to 30 nm. The CA, ZnO and CA-ZnO composite materials were characterized by FT-IR SEM, EDX, and XRD. The photocatalytic process involved the degradation of methyl orange (MO) under UV light conditions and it was highly influenced by the morphology of the CA-ZnO composite.

Audience Take Away:

- The use of biomass residues in order to create future added-value products based on CA
- The synthesis of composite materials with higher efficiency in the field of photocatalytic degradation process for contaminated waters
- The ease of recovery of the CA-ZnO composite materials by improvement of separation process
- The possibility to reuse the CA-ZnO composite materials in a new photodegradation cycle.

CONTENTS

Biography

Alexandra Mocanu is currently an Assistant Professor at the Department of Chemical and Biochemical Engineering, Faculty of Applied Chemistry and Materials Science, University POLITEHNICA of Bucharest, Romania. In 2012, she obtained her PhD title in Chemical Engineering for "Self-assembled polymer colloidal dispersions". Her research field involve polymer photonic crystals, synthesis and characterization of inorganic particles by conventional and unconventional methods (ultrasound and microwave-assisted reactions), wastewater treatment, chemical reconversion of plastic and biomass wastes, formulations for polyurethane products (adhesivez, foams, resins, etc.). She published over 40 papers in journal indexed by ISI and participated to over 25 international conferences.

Electrochemically derived Poly-porphyrin films with electrocatalytic properties

Vladimir Ivanovich Parfenyuk*[1,3], Svetlana A. Chulovskaya[1], Sergey M. Kuzmin[1,2], Mariya V. Tesakova[1]
[1]G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences, Ivanovo 153045, Russia
[2]Ivanovo State Power Engineering University, Ivanovo 153003, Russia
[3]Ivanovo State University of Chemistry and Technology, Ivanovo 153000, Russia

The fundamental and applied interest in natural porphyrins and their synthetic analogues is related to the possibility of obtaining porphyrin-based materials. They have various functional properties which can vary due to the molecular interacting and substitutes.

We present electrocatalytic films of ClFe(III)5,10,15,20-tetrakis(p-aminophenyl) porphyrin (FeClT(p-NH_2Ph)P) formed by new electrochemical deposition method using oxygen saturated dimethyl sulfoxide solutions (DMSO) as a medium. Superoxide promotes the poly-porphyrin film formation on the working electrode surface due to it high affinity both to hydrogen atom and to proton. The most favorable pathway of the superoxide-assisted electrochemical polymerization is proposed. The resulting poly-FeClT(p-NH_2Ph) P films are smooth, golden colored, well adhesed with substrate and quite insoluble in water, ethanol and dichloromethane. The film formation accompanied with broadening and red-shifting of the Soret band. Atomic force microscopy (AFM) investigation shows homogeneity, low roughness and nanoscale globular structure of the poly-FeClT(p-NH_2Ph)P films.

The poly-FeClT(p-NH_2Ph)P films obtained on glassy carbon were studied for electrocatalytic activity in the reaction of electrochemical reduction of oxygen in an alkaline medium. Current densities about 0.1 mA/cm^2 are recorded near -0.2 V while the potential is cycled on the glassy carbon in the degassed 1 M solution of KOH (Fig., curves 1). It can be related to the incomplete removal of oxygen from the solution. An irreversible wave of electroreduction of oxygen with a current density of about 0.42 mA/cm^2 is detected when the solution is saturated with oxygen (Fig., curves 2). The oxygen electroreduction onset on glassy carbon is close to 0 V vs. Ag/AgCl electrode. The maximum of the electrochemical response of the oxygen electroreduction is localized in the potential region (-0.2÷-0.3 V). For the electrodes modified by the poly-FeClT(p-NH_2Ph)P film the potential of the oxygen electroreduction onset is shifted to the positive region by 0.14 V(Fig., curves 3). The intensity of the current density peak of the oxygen electroreduction increases. The films obtained from DMSO solutions have a sufficiently smooth surface and do not significantly change the capacitance of the working electrode. It is indicated by the same value of current densities at the initial and modified electrodes under polarization in the potential range 0.2÷0.7 V. Consequently the set of changes in the response of the electrochemical reduction of oxygen indicates the electrocatalytic activity of the poly-FeClT(p-NH_2Ph)P film.

Working ability of the electrode modified by polyporphyrin film was tested by repeated cycling under the conditions of the electrocatalytic process. It was found that for more than 20 cycles the electrochemical response of the oxygen electroreduction remains unchanged. After removal from the cell, the film retained its original form.

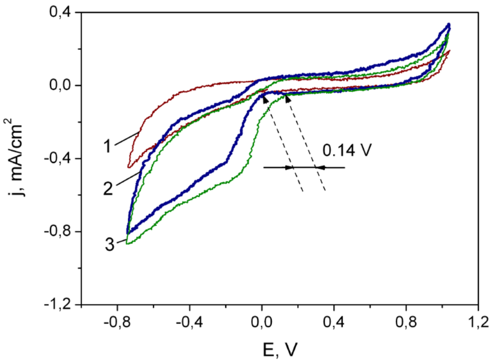


Fig. CV of O2 reduction in aqueous alkaline media at glassy carbon electrode in degassed (1) and O2 saturated (2) solutions; at poly-FeClT(p-NH2Ph) P modified glassy carbon electrode in O2 saturated solution (3). The potentials are measured vs Ag/AgCl, the scan rate is 0.02 V/s.

Polyporphyrin films are a new class of electrically conducting polymers with semiconductor properties. These materials can be used as elements of solar batteries, sensors, catalysts, etc. The electrochemical method of production allows controlling the properties of films by changing the electrolysis modes, the nature of the solvent and the nature of the porphyrin monomer.

CONTENTS

Biography

Parfenyuk Vladimir Ivanovich, Doctor of Chemical Sciences, Professor, Chief Researcher of the Institute of Solution Chemistry Russian Academy of Sciences, Professor of the Department of Chemistry Kostroma State University, Professor of the Department of Electrochemistry Ivanovo State University of Chemical Technology. Head of the scientific group engaged in scientific research in the field of electrochemistry of organic and inorganic compounds, plasma chemistry, physical chemistry of solutions. Author of more than 400 scientific papers. He has extensive experience in scientific and organizational work in the area of preparation and conduct of scientific events. Since 2008 year - Organizer and Chairman of the Organizing Committees of the International Conferences "Modern Methods in Theoretical and Experimental Electrochemistry" (Ples Russia), "New Functional Materials and High Technologies" (Tivat, Montenegro), member of the Organizing Committees of the International Conferences "Electrochemical and Electrolytic Plasma Methods for Modifying Metallic Surfaces" (Kostroma, Russia), "Theory and practice of modern electrochemical production" (St. Petersburg, Russia), etc.

Parfenyuk V. – the member of International Society of Porphyrins and Phthalocyanines (SPP), International Association of Advanced Materials (IAAM), has been honored with prestigious IAAM Medal (Stockholm, Sweden 2017).

Photoactivity of ZnO supported MCM-41

Duygu Tuncel*, Ayşe Neren Ökte
Boğaziçi University, Turkey

Mesoporous molecular sieves like silica of the MCM-41 type exhibit well-ordered structure with highly controlled cylindrical channels and very narrow pore size distributions. With large specific areas, controllable pore size and homogenous structure, the material has potential applications in various fields. In addition, mesoporous materials of the MCM-41 type are superb candidates in mitigating the urban thermal pollution through the cycle of water vapor adsorption-condensation-evaporation-desorption due to their hydrophilicity and capillary condensation effects in their nanopores. Also, there are only a few studies where semiconductor nanoparticles incorporated in the mesoporous solid MCM-41.

In this study, silica source from a hydrothermally treated low cost mineral was used to prepare hydrophilic mesoporous material by the sol-gel technique and test for water vapor adsorption and pollutants photodegradation. The prepared material as well as a commercial MCM-41 were used as hosts for the formation of ZnO-MCM-41 composite. The as-synthesized composite was characterized by X-ray diffraction (XRD), Scanning electron microscopy (SEM) images with energy dispersive X-ray analysis (EDX) coupled with elemental mapping scans, (UV-VIS-NIR) absorption spectroscopy, nitrogen adsorption desorption (BET)and water vapor adsorption isotherms. The photocatalytic activity for the degradation of methyl orange (MO). The high efficient removal of MB by the hydrophilic composites combined with their alternative preparation from low-cost raw silica expands their application prospects for combined energy and environmental applications.

Audience Take Away:

As preliminary experiments and baseline information:

- Determination of photocatalytic degradation of organic pollutants
- Determination of physico-chemical properties of photocatalyst,

Understanding of the physico-chemical behavior of the reacting partners:

- Application of specific physico-chemical methods, i.e. surface area and pore size distribution, particle size calculations,
- Application of adsorption and photocatalytic degradation systems

Biography

Duygu Tuncel obtained her B.S. in Chemistry from the Chemistry Department of Yıldız Technical University in 2012. She received her M.Sc. degree entitled as “TiO2 and ZnO Loaded Fly ash Catalysts” from the Chemistry Department of the Institute of Graduate Studies in Sciences and Engineering of Boğaziçi University in 2014. Currently, she is a Ph.D. candidate and Teaching Assistant at the Institute of Graduate Studies in Sciences and Engineering of Boğaziçi University. Her research interests include preparation and activity testing of novel photocatalysts based on metal organic frameworks, adsorption and photocatalytic degradation applications, humidity applications.

Hydrothermal synthesis of [Al]ZSM-5 and [Ga]ZSM-5 type zeolites

Totka Todorova[1]*, **Yu. Kalvachev**[2]
[1]Institute of Mineralogy and Crystallography, Bulgarian Academy of Sciences, Acad. G. Bonchev St., bl. 107, 1113 Sofia, Bulgaria
[2]Institute of Catalysis, Bulgarian Academy of Sciences, Acad. G. Bonchev St., bl. 11, 1113 Sofia, Bulgaria

Zeolites are crystalline aluminosilicates, composed of TO_4 tetrahedra (T = Si, Al) with O atoms connecting neighboring tetrahedral, that contain pores and cavities of molecular dimensions. Many occur as natural minerals, but it is the synthetic varieties which are among the most widely used sorbents, catalysts and ion-exchange materials in the world. The isomorphous substitution of Si^{4+} or Al^{3+} by Ga^{3+} is interesting from practical point of view. Catalytic processes for fine chemical productions and oxidation reactions are amenable to the employment of tuned and novel zeolites. The phenomenon of isomorphous substitution is well-known in the field of mineralogy. By isomorphous substitution, framework atoms of crystalline compounds are replaced by atoms of other elements without changing the type of the crystal structure.

This study reported on the hydrothermal synthesis of AlZSM-5 and GaZSM-5 zeolite from systems containing tetrapropylammonium bromide as an organic structure determining agent. The crystallization conditions were optimized by varying the heating time for both systems. AlZSM-5 was obtained from a system $50SiO_2 : Al_2O_3 : 5.0Na_2O$: 5.0TPABr : 2000H2O after 72 hours at a crystallization temperature 170oC. Pure GaZSM-5 is obtained from an initial gel 30SiO2 : $Ga_2O_3 : 4.4Na_2O$: 18TPABr : $1000H_2O$ after 114 hours and crystallization temperature 150°C. Post synthesis treatment is applied in order to increase the specific surface area and providing easy access to the active zeolite centers. Secondary pores in crystals were formed by etching at room temperature with solution of NH4F and 0,25M HF acid, varying the time of treatment. All samples have been characterized by X-ray diffraction analysis, scanning electron microscopy (SEM), infrared spectroscopy (IR), solid-state nuclear magnetic resonance (NMR) spectroscopy and physical absorption-desorption of nitrogen.

Biography

T. Todorova graduated Bachelor and Master degree in Faculty of Chemistry and Pharmacy, Sofia University "St. Kliment Ohridski" - Sofia, Bulgaria. In 2015 I finished my PhD thesis with title “Synthesis optimization of zeolites type pentasyle” with supervisor Prof. Yu. Kalvachev in the Institute of Mineralogy and Crystallography “Acad. Ivan Kostov” – Bulgarian Academy of Sciences. During my studies I have held different positions as: laboratory assistant, chemist specialist, assistant professor and currently I hold a permanent position as chief assistant professor at the same institute. Until now I have 7 articles, 5 of which are published in international impact factor journals. I have participated in 10 scientific forums and 8 projects. During my training, I had the pleasure to work with Prof. D. Sc. G. Vayssilov, Prof. Yu. Kalvachev, Assoc. Prof. L. Dimitrov and Prof. V. Valtchev.

CONTENTS

Nanostructure control of IrO_x powder for highly efficient electrocatalytic water oxidation

Tetsuya Sato*, Kenji Saito, Tatsuto Yui, Masayuki Yagi
Niigata University, Japan

Widespread attention has recently been paid to artificial photosynthesis as a promising energy-providing system for the future to produce green and storable hydrogen fuel. The efficiency of hydrogen generation from photoelectrochemical and electrochemical water splitting is severely limited by the sluggish kinetics of oxidation of water. Therefore, the development of efficient electrocatalysts for water oxidation is an avenue to improve the competence of a fuel generation technology. Iridium oxide (IrO_x) catalysts have been widely studied for water oxidation in both electrochemical and photochemical systems, owing to its actuation over a broad pH range, low resistivity, and superior chemical/thermal stability. Nanostructure control of IrOx is important to develop high activity water oxidation catalyst based on IrO_x. We reported the formation of a mesoporous IrOx thin film using an amphiphilic block polymer as a template, which has a high specific surface area (105 m^2g^{-1}). IrOx powder is widely used, but IrO_x powder having a specific surface area of 100 m^2g^{-1} or more has not been developed so far. Herein we report to create IrO_x powders with a high specific surface area without using templates.

Biography

Tetsuya Sato graduated from Niigata University (Japan) in 2018 and went on to graduate school in Niigata University.

Influence of chemical states of doped nitrogen in $NaTaO_3$ on photocatalytic activity for CO_2 reduction

Akiyo Ozawa[1]*, Keita Kobayashi[2], Tomoko Yoshida[3]
[1]Osaka City University, Sakai Chemical Industry, Co., Ltd., Japan
[2]Sakai Chemical Industry, Co., Ltd., Japan
[3]Osaka City University, Japan

Reduction of CO_2 in atmosphere is an important environmental issue, and photocatalytic conversion of CO_2 to useful compounds like CO has been studied extensively. As Nakanishi et al. reported, $NaTaO_3$ shows high photocatalytic activity for CO_2 reduction and attracts much attention. However, owing to its rather wide gap nature (4.1ev), $NaTaO_3$ shows the photocatalytic activity only under UV light irradiation up to 300 nm in wavelength region which corresponds to about 1.7×10-4 % in the total solar energy. If NaTaO3 exhibits the photocatalytic activity under visible light, for example, up to 350nm, the usable solar energy will increase about 5000 times, 0.89% in total solar energy. Therefore the band gap narrowing of $NaTaO_3$ is encouraged. Although nitrogen doping into $NaTaO_3$ could narrow its band gap from 4.1 eV to 2.2 eV, the effects of the nitrogen doping on photocatalytic CO2 reduction of $NaTaO_3$ have not been studied well. In this study, nitrogen doped $NaTaO_3$ was synthesized by a solid state reaction or hydrothermal reaction to investigate the relationship between chemical states of doped nitrogen and the photocatalytic activity of the samples.

In the solid state reaction, nitrogen doping was done under NH_3 flow at 1223 K for 7 hours on $NaTaO_3$ synthesized as precursor in advance, resulting red colored powders. Analyses of the powders by XPS, XANES and UV-vis showed no nitrogen doped.

In the hydrothermal reaction, Ta_3N_5 and NaOH aqueous solution were reacted under hydrothermal condition giving orange colored powders. It was confirmed that nitrogen was doped in the powders. The amount of doped nitrogen could be controlled by changing the mixing ratio of Ta_3N_5 and NaOH. The nitrogen doped $NaTaO_3$ is referred as $NaTaO_{3-x}N_x$ hereafter. Depth distribution of the doped nitrogen was determined by XPS analysis under stepwise Ar sputtering. The concentration of the doped nitrogen was highest at the surface and decreased with depth showing deeper penetration in the particles having higher surface concentration.

The synthesized $NaTaO_{3-x}N_x$ samples were modified by Ag nanoparticles as cocatalyst, and their activities on photocatalytic CO_2 reduction under UV light or visible light irradiation were examined. Unfortunately, the photocatalytic CO_2 reduction under visible light irradiation did not proceed. Under UV light irradiation, $NaTaO_{3-x}N_x$ showed higher activity for the CO_2 reduction than $NaTaO_3$. In the anodic photocurrent measurements under UV light irradiation, $NaTaO_{3-x}N_x$ showed higher anodic photocurrent corresponding with their higher activities on the CO_2 reduction. Different from the UV irradiation the anodic photocurrents of $NaTaO_{3-x}N_x$ under visible irradiation monotonously increased with increasing nitrogen content (x). This result suggested that the amount of electron-hole pairs generated by visible light irradiation depends on the amount of doped nitrogen in $NaTaO_3$.

Audience Take Away:

- How to control the amount of doped nitrogen in $NaTaO_3$ in hydrothermal synthesis.
- Methods to get depth distribution of doped nitrogen in $NaTaO_3$ and their chemical states.
- Correlation among photon absorption, anodic photocurrent and photocatalytic activity of nitrogen doped $NaTaO_3$.

Biography

Akiyo Ozawa is a graduate student in doctor course in Osaka City University (OCU) in Japan, She is currently working on developing $NaTaO_3$ photocatlyst to use for CO_2 reduction. She got student award in 11th International Symposium on Atomic Level Characterizations for New Materials and Devices '17 in 2017. After graduating master course in OCU, she has been working in Sakai Chemical Industry Co. Ltd. in Japan. She is greatly contributing on the research and development of phosphors materials to apply to plasma panel displays. In 2016, she joined to professor Yoshida' group in OCU to conduct research for photocatalytic CO_2 reduction.

Effect of surface-modified Silica/ Polyamideimide (PAI) films

Hohyeong Kim, Heungyeol Lee, Jae Young Park*, Ph.D.
Korea Institute of Industrial Technology, Republic of Korea

Winding wire is composed of copper (Cu) core enclosed by an insulation coating layer. Specially, Polyamide-imide (PAI) of several kinds polymers has been used in various fields such as mechanical strength, electrical conductivity, high thermal stability and dielectric constant. Silica nanoparticles have a hydrophilic surface and high surface energy leading to low compatibility with hydrophobic polymer. When the silica and PAI are prepared, some mechanical properties of the composite such as the elongation at break point were rather poor as the silica content was increased.

In this work, to overcome this problem, the key was how to improve the compatibility of the silica nanoparticles with PAI and maintain the good dispersion stability of silica nanoparticles within PAI films. The surface modification is the most widely used method using a silane coupling agent (SCA) which contained amino-, expoxy group. After the surface modification process, the modified silica nanoparticles had the better compatibility with PAI matrix and the modified silica nanoparticles could be well dispersed into the PAI matrix, even when the amount of silica to PAI reached to 5 wt%. Electric resistance properties of the nanocomposite winding wire were investigated.

Biography

Jae Young Park joined Research Institute of Advanced Manufacturing Technology, Surface R&D Group, Korea Institute of Industrial Technology (KITECH), in 2010 as a senior researcher. He received his B.S. and M.S. degrees from the Chonnam University, Republic of Korea in 2003 and 2005. In 2010, He received his Ph.D. from Inha Univerisrty, Republic of Korea. He joined as a Post-doctoral fellow at the Inha Uni-versity in 2010. He has been working on metal oxide gas sensors synthesized by the sol–gel process, electrospinning and VLS method.

Sol-gel synthesis of $MgFe_2O_4$ nanoparticles for photodegradation application

Gulzat Demeuova*, Aliya Kurbanova, Ozhet Mauit, Ph.D., Murat Baisaryev, Oral Ualibek, Ph.D., Olzat Toktarbaiuly, Ph.D., Gulnar Sugurbekova
PI National Laboratory Astana, Kazakhstan

Water purification and environmental remediation has been one of critical issues arising with increasing demand for portable water. Industrial effluents, primarily synthetic colourings from textile dyes such as methylene blue contribute predominantly to water pollution. Therefore, the aim of this study was to investigate efficient degradation of methylene blue under solar light irradiation employing magnesium ferrite photocatalysts synthesised by two way sol gel technique, where target was to obtain nanoparticles with the maximum content of specified ferrites, uniform particles with high crystallinity. In the first method, $MgFe_2O_4$ nanoparticles were synthesized by co-precipitation of magnesium and iron hydroxides, whereas second sol-gel method is based on magnesium acetate and iron nitrate precursors. For both methods annealing was performed at 400-600ºC for growth of magnetic nanoparticles. Structure and morphology of $MgFe_2O_4$ nanoparticles were characterized by XRD and SEM. According to XRD pattern, 100% spinel ferrite with crystallinity of 77.6% has been achieved at pH=7.0 and showed most uniform particle size distribution with crystallite size of 10-50 nm. Nanoparticles obtained using second method showed phase content of Fe_2O_3 23.8% and $MgFe_2O_4$ 76.2% with crystallinity of 74.3%. The photocatalytic experiments performed under solar light irradiation showed, total degradation of MB with $MgFe_2O_4$ obtained from first method in 2 hours and 15 min at concentration 0.4 g/L of photocatalyst. It is one of the promising photocatalysts for waste water treatment.

Biography

Gulzat Demeuova is a junior researcher in Laboratory of Materials Processing and Applied Physics at Center for Energy and Advanced Materials Science founded at Nazarbayev University. She received her MSc in Chemical Engineering from University of Leeds, UK and BSc in Chemical Engineering from University of Bath, UK in 2014 and 2010 respectively. Her research background orients from cyanide leaching of gold, hydrophobic materials, photocatalysis for water treatment and GaN thin films. Results of her work are formed in patent and publications in international and local journals.

Photocatalytic activity of surface modification of TiO_2 nanoparticles

Hohyeong Kim*, Heungyeol Lee, Jae Young Park, Ph.D.
Korea Institute of Industrial Technology, Republic of Korea

TiO_2 is of interest for various applications such as photocatalytic, photoelectrochemical, and super-hydrophilic properties. However, TiO_2 nanoparticles are very easily to agglomerate in mediums and show poor dispersion capacity in solvents, and therefore the applications of TiO_2 nanoparticles are mainly limited. Surface modification of TiO_2 nanoparticles is an important pathway toward the synthesis of hybrid materials. The main application of these hybrid materials are synthesis of polymer composite due to the enhanced phase compatibility and formation of ordered structures by controlled self-assembly and improvement of dispersibility of the nanoparticles in various media.

In this works, For the improvement of TiO_2 nanoparticles dispersion, the surface of TiO_2 nanoparticles was modified with Amino- silane coupling agent (SCA). The goal of this work was to synthesize modified TiO_2 nanoparticles using surface modification method, and to establish optimal synthetic parameters. The microstructure and properties such as self-cleaning, surface hydrophobicity, ultraviolet and corrosion resistance were investigated.

Biography

Hohyeong Kim joined Research Institute of Advanced Manufacturing Technology, Surface R&D Group, Korea Institute of Industrial Technology (KITECH), in 2009 as a researcher. He received his B.S. and M.S. degrees from the Inha University, Republic of Korea in 2007 and 2009. He has been working on metal oxide gas sensors and on the synthesis of metal nanoparticles.

Titanium based catalyst systems for photo-catalytic CO_2 reduction

Aigerim Baimyrza*, Mannix Balanay, Ph.D., Moulay-Rachid Babaa, Ph.D., Zhumabay Bakenov, Ph.D.
Nazarbayev University, Kazakhstan

The development of facile and robust photo-catalyst to establish the photo-catalytic CO_2 reduction in industrial scale firstly would considerably reduce the amount of greenhouse gases in the atmosphere; secondly, it would found a renewable source of industrially valuable compounds like methanol, formic acid and other hydrocarbon compounds.

Ti-based compounds including TiO_2 remains to be the most robust photo-catalyst for CO_2 reduction with two main drawbacks: poor selectivity and high activation energy. Incorporation of vanadium with titanium in ternary metal oxides considerably narrows the band gap energy from 3.2 eV for pure TiO_2 up to 1.7 eV for Ti-V-O ternary oxide with the increase of vanadium content, making the ternary oxide visible light active. Ti-based MOFs are an ideal class of materials to apply as a catalyst for the range of photo-catalytic processes including the photo-reduction of CO_2. Introduction of Ti into MOF may allow to tune the photo-responsive properties and selectivity of titanium and enhance other properties of the catalyst as the porosity and stability by changing the organic counterpart.

Herein we report on $Ti_xV_yO_z$ and new type Ti-MOF composites and their photo-catalytic properties. The obtained composites were characterized by XRD, TEM, SEM, BET and TGA. The CO_2 conversion rate was also studied by changing reaction parameters such as UV wavelengths, gas flow rate, etc.

Audience Take Away:

- Properties of new catalysts will be presented.
- Information about properties and advantages of new catalysts will allow participants to evaluate if presented catalysts can be applied to their reactions.
- Drawbacks of earlier and recently applied catalyst systems for the reaction will be introduced and according to this information other participants can evaluate if their catalytic systems can be applied to the reaction.

Biography

Aigerim Baimyrza hold a BTech degree in Chemical Engineering of Organic Substance from Al-Farabi Kazakh National University and MSc degree in Polymer Material Science and Engineering from University of Manchester. After the graduation she joined Nazarbayev University (Astana, Kazakhstan) as a Teaching Assistant and the Institute of Batteries (Astana, Kazakhstan) as a Junior Researcher. Currently she is a Research Assistant in Nazarbayeve University and a part of research team working on photo-catalytic conversion of CO_2 into hydrocarbon fuel.

CONTENTS

Oxidative carboxylation of 1-decene

Raiedhah Alsaiari*, Rebecca V. Engel, Ewa Nowicka, Graham J. Hutchings
Najran Univeristy, Saudi Arabia

This work reports a direct route for the synthesis of cyclic carbonate starting from terminal alkene, which avoids the preliminary synthesis and isolation of terminal epoxide. A catalyst system consisting of Au/support, tetrabutylammonium bromide (Bu_4NBr) and zinc bromide ($ZnBr_2$) has been applied to the one-pot synthesis of cyclic carbonate from 1-decene, O_2 as primary oxidant, and CO_2. Supported gold catalyst is active for the epoxidation of 1-decene, and zinc bromide and Bu4NBr catalyse the subsequent CO_2 cycloaddition to epoxide. The influence of various reaction parameters, such as CO_2 pressure, reaction temperature, reaction time, catalyst preparation methods and catalyst amount, has been studied in more detail. It should be noted that under this reaction system, no need for an organic solvent, a high reaction temperature, or high CO_2 pressure.

Audience Take Away:

- Utilization of carbon dioxide
- Direct synthesis of cyclic carbonate starting from low price alkene instead of an expensive epoxide under solvent-free conditions.

Biography

Assistant professor at Najran university Saudi Arabia, graduated from king Saudi university, I had got the MSc and PhD from Cardiff university in the catalysis. Published 3 papers.

Synthesis and characterization of bimetallic Ce Zr based UiO-66 and MOF-808

Michalina Stawowy*, Janusz Trawczyński, Agata Łamacz, Ph.D.
Department of Fuel Chemistry and Technology, Wrocław University of Science and Technology, Gdańska 7/9, 50-344 Wrocław, Poland

Metal Organic Frameworks (MOFs) are relatively new group of porous, crystalline materials with three - dimensional structure. They are composed of metallic cluster connected with organic ligand. The UiO-66 and MOF-808 (both containing Zr) have excellent chemical, thermal and mechanical stability but Zr^{4+} cations are weak Lewis acids so exchanging part of Zr cations with Ce could improve their adsorptive and catalytic properties. Cerium characterizes with very good redox properties; hence introduction of those cations to UiO-66 or MOF-808 should enhance CO_2 adsorption owing to Ce^{3+} presence.

The aim of our work is the synthesis of bimetallic Ce/Zr-MOFs with UiO-66 and MOF-808 topology. We investigated the influence of synthesis parameters on their properties. Ce/Zr-UiO-66 and Ce/Zr-MOF-808 were obtained via solvothermal method in a Teflon-lined autoclave. Organic linker (benzene-1,3,5-tricarboxylic acid or benzene-1,4- dicarboxylic acid) and metals precursors ($ZrO(NO_3)_2 \cdot XH_2O$ and $(NH_4)_2Ce(NO_3)_6$) were dissolve in N,N- dimethyloforamide (DMF) and then kept at 120 °C for 0.5, 24 and 72 h. After washing with DMF and filtering off, the DMF was exchanged with chloroform. Obtained materials were dried at 120 °C for 12 h.

The structure, composition, textural properties and thermal stability of Ce/Zr-UiO-66 and Ce/Zr-MOF-808 were determined using XRD, XPS, IR, N_2 sorption, SEM and TGA. The CO_2 sorption capacity of these materials was also determined.

Audience Take Away:

- How the synthesis parameters influence the physico-chemical properties of Ce/Zr based MOFs
- How the composition of MOFs influences their CO_2 adsorptive properties.

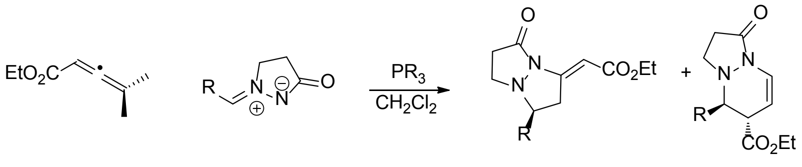
Biography

Michalina Stawowy is a PhD student in the Department of Fuel Chemistry and Technology at the Wrocław University of Science and Technology. Her field of interest are new cerium containing mono-, bi- and polymetallic MOFs for carbon dioxide adsorption and its catalytic conversion e.g. to methanol.

On the mechanism of phosphine-catalyzed annulation of azomethine imines with allenoates: Theoretical insights

Sebastián Gallardo-Fuentes[1], Ph.D., Patricio Fuentealba[2], Prof. Dr.
[1]Departamento de Química, Facultad de Ciencias, Universidad de Chile, Casilla 653, Santiago, Chile
[2]Departamento de Física, Facultad de Ciencias, Universidad de Chile, Casilla 653, Santiago, Chile

In the search of new chemical processes with benign environmental impact, the organocatalyzed reactions have become a powerful alternative to the well-known metal-catalyzed reactions. A remarkable feature inherent to organocatalytic reactions is the biomimetic nature in which these catalysts enhance or modify the intrinsic reactivity of a substrate, often forming a covalent catalyst-substrate complex that resembles the enzymatic-machinery. In this line, the unique reactivity of phosphines compared to amines has enabled the development of new and unprecedented reactivity patterns. In phosphine-catalysis, the key step involves the formation of a catalyst-substrate complex through a nucleophilic attack of the phosphorous atom onto the substrate, commonly an electrophilic π-compound. Even though a lot of phosphine-catalyzed annulation reactions have described in the past few years, theoretical studies devoted to the mechanism of these transformations are yet scarce. For this reason, in this work we describe the potential energy surface of the PMe3-catalyzed [3+2] annulation of allenoate 1 with azomethine 2 as model reaction (Scheme 1), in order to elucidate the reactivity patterns and the selectivity outcome in these processes. To unravel the origins of regioselectivity patterns we analyzed the reaction pathways associated to the nucleophilic addition of phosphonium-dienolate intermediate to azomethine imine 1 by means of local hard–soft acid–base (HSAB) principle and non-covalent index (NCI). Because the final step in phosphine-catalyzed cycloaddition involves a ring-closing step followed by a proton-transfer/phosphine-departure sequence, the next issue worth examining is the assessment of the role of stereoelectronic effects at the cyclization step. The results obtained emphasize the role of the tether strain and steric effects present at the ring-closing step. Finally, both the role of general-base mechanism in proton transfer step and the nucleofugality of phosphine along the cyclization step are also discussed. The insights presented herein can be used as a key piece of information to inspire the design of other phoshine-catalyzed cycloaddition reactions.



1 **2** **3** **4**

Scheme 1: Phosphine-catalyzed cycloaddition of allenoates 1 with azomethine imine 2.

Audience Take Away:

This presentation gives useful insights for rational catalyst design purpose as follows:

- Unraveling the origins of regio- and diasteroselectivity patterns in phosphine-catalyzed cycloadditions
- Elucidating the role of stereoelectronic effects on the reaction outcome at the cyclization step
- Providing insights to understand the role of electronic structure of the catalyst along the reaction pathway

Biography

Sebastián Gallardo received his Ph.D. degree in Chemistry from the Universidad de Chile in 2016 under the supervision of Professor Renato Contreras. His research interests center on the elucidation of selectivity patterns in tandem reactions by means of computational tools. He currently works as a postdoctoral researcher under the direction of Professor Patricio Fuentealba where he is focusing on the elucidation of reaction mechanism and selectivity patterns in phosphine-catalyzed cycloaddition with aid of quantum chemical topological analysis.

DAY 1

E-POSTERS

2nd Global Conference on

Catalysis, Chemical Engineering & Technology

SEPTEMBER 13-15, 2018
ROME, ITALY

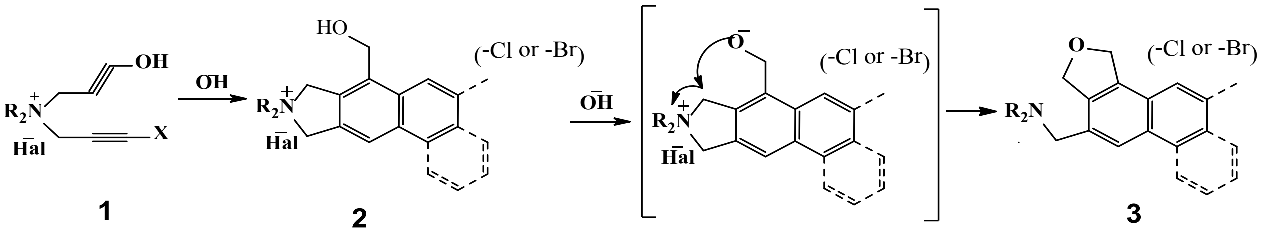
CONTENTS

Base catalized intramolecular cyclization of -(4-hydroxybuth-2-ynyl)[3-(4-aryl) prop-2-ynyl]ammonium chlorides and intramolecular recyclization of obtained products

Chukhajian E. O.[1]*, Ph.D., Shahkhatuni K. G.[1], Ph.D., Chukhajian El.O.[1], Ph.D., Gevorgyan H.R.[1], Ph.D., Khachatryan A. A.[2], Ph.D.

[1]The Scientific Technological Centre of Organic and Pharmaceutical Chemistry of National Academy of Sciences of Republic of Armenia
[2]Gyumri State Pedagogical Institute after M. Nalbandyan

It was established that for Cyclization of -(4-hydroxybuth-2-ynyl)[3-(4-aryl)prop-2-ynyl]ammonium chlorides (1) in the presence of 0,2 mol of alkali per mol of initial salt, unlike of propargylyc analogs [1], it is necessary the heating of reaction mixture at 45-50oC during 10-15 min, then take place Cyclization with self-heating giving cyclic products (2) with high yields.



X= Ph, 4-CH_3Ph, 4-Cl-(or -Br)Ph, α–naphthyl

In these conditions with 13-15% yields were obtained also amines 3, which are result of intramolecular Recyclization of cyclic products 2.

It was shown that the Cyclization of dialkyl(4-hydroxybuth-2-ynyl)[3-(4-bromphenyl)prop-2-ynyl]ammonium chlorides in water medium at step addition of twofold mol of water base on one mol of initial salts is realized with self-heating and following Recyclization of cyclic products 2, leading with high yields to formation of amines of Recyclization 3.

The chlorides of 2,2-pentamethylene-6-brombenzo[f]isoindolinium and (spiro-6-brombenzo[f]isoindolin)-2,4'-morpholinium in water solution at room temperature in the presence of equimolar quantity of KOH smoothly undergo intramolecular Recyclization with formation of amines 3 with high yields.

The observing phenomenon is unique case in the field of intramolecular Recyclization. This can be explained by the fact that in the presence of bromine atom in the cycle is increased the electronic density of the molecule, thereby facilitates the ability of nucleophilic attack of alkoxy anion on a partially positive charged isoindolinium cycle.

Audience Take Away:

- From this presentation the audience will learn how to expand the area of base catalized intramolecular Cyclization and Recyclization which include huge possibilities for synthesis of new bioactive nitrogen-containing heterocycles, 1,3-dihydrobenzofurans and their condensed analogs.
- These compounds have proved to be very attractive and useful for the synthesis and design of molecules of potential drugs.

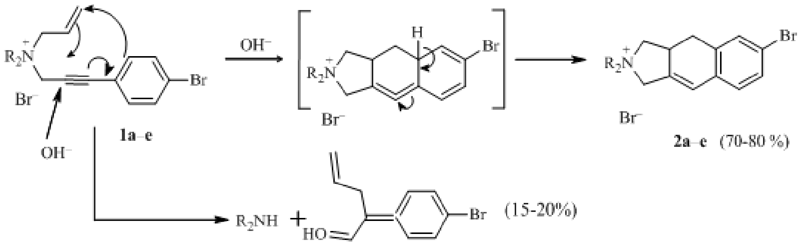
Biography

Prof. Emma Chukhajian is Leading Scientist and Head of the laboratory of aminocompounds of The Scientific Technological Centre of Organic and Pharmaceutical Chemistry of National Academy of Sciences of Republic of Armenia. She obtained her Ph.D. in Science in 1970 and postdoctorial in the group of Academician Araksya T. Babayan. In 1969 with A. Babayan she discovered base-catalized intramolecular Cyclization of unsaturated ammonium salts containing β,ϒ-unsaturated groups along with 3-alkenyl(aryl)propargylic groups. In 2003 she with coauthors revealed intramolecular Recyclization of 4-hydroxymethylisoindolinium salts and their condensed derivatives. Among of cyclic products there are representatives with pharmacological activity. In 2008 – the phenomenon of isomerisation of 3a,4-dihydroisoindolinium salts, in 2011 – that Stevens rearrangement of the salts, containing allylic type group along with 4-hydroxybuth-2-ynyl, includes the stages of simultaneously transfer of reaction centre in accepting group and conversion of migrating group, in 2016 – phenomenon of deamination during vacuum distillation of 3-(dialkylamino)-1,4-diarylhex-5-en-1-yns and was worked out the method of preparation of terphenyle and its derivatives.

Base catalized intramolecular Cyclization of –allyl[3-(4-bromphenyl)prop-2-ynyl] ammonium bromides and water-base cleavage reaction of obtained cyclic products

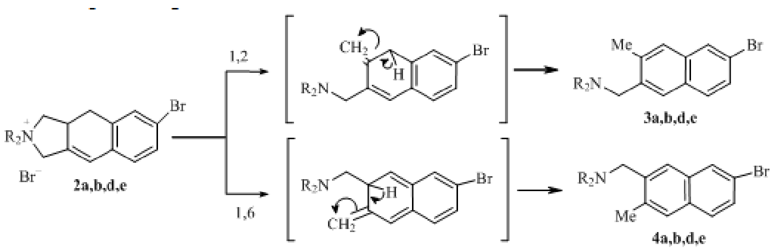
Chukhajian E.O.[1]*, Ph.D., Ayrapetyan L. V.[1], Ph.D., Mkrtchyan H. S.[1], Sargsyan M. H.[2], Ph.D.
[1]The Scientific Technological Centre of Organic and Pharmaceutical Chemistry of National Academy of Sciences of Republic of Armenia
[2]Gyumri State Pedagogical Institute after M. Nalbandyan

It was established that for Cyclization of salts 1 a-e in the presence of base in mole ratio salt/base 5/1, in contrast to propargylic analogs [1,2], need to be heating reaction mixture at 90 0C for 2 h. In these conditions along with Cyclization, which is the main direction, take place also rearrangement-cleavage reaction leading to formation of corresponding secondary amines and 1-allylcinnamaldehyde.



1,2 a R = Me, **b** R = Et, **c** R_2 = –$(CH_2)_4$–, **d** R_2 = –$(CH_2)_5$–, **e** R_2 = –$(CH_2)_2O(CH_2)_2$–

It is shown that cyclic products 2 a-e rather smoothly undergo water-base cleavage reaction in the directions of 1,2 and 1,6. In the results were formed the mixture of isomer amines 3 a,b,d,e and 4 a,b,d,e with 57-60 % overall yields. According to NMR H1 and C13 the mixture is composed of the two isomer amines with different percentage ratio.



3,4 a R = Me, **b** R = Et, **d** R_2 = –$(CH_2)_5$–, **e** R_2=–$(CH_2)_2O(CH_2)_2$–

Audience Take Away:

- From this presentation the audience will learn that base catalized intramolecular Cyclization of new unsaturated ammonium salts gives the large possibilities for synthesis of new bioactive derivatives of -benzo[f]isoindolinium and 3a,4-dihydrobenzo[f]isoindolinium salts, compounds, the synthesis of which by other chemical ways is unaccessible.
- The expanse of the field of water-base cleavage reaction of -dihydrobenzo[f]isoindolinium salts leads to formation of new bioactive derivatives of dialkylaminomethylnaphtalines.

Biography

Prof. Emma Chukhajian is Leading Scientist and Head of the laboratory of aminocompounds of The Scientific Technological Centre of Organic and Pharmaceutical Chemistry of National Academy of Sciences of Republic of Armenia. She obtained her Ph.D. in Science in 1970 and postdoctorial in the group of Academician Araksya T. Babayan. In 1969 with A. Babayan she discovered base-catalized intramolecular Cyclization of unsaturated ammonium salts containing β,ϒ-unsaturated groups along with 3-alkenyl(aryl)propargylic groups. In 2003 she with coauthors revealed intramolecular Recyclization of 4-hydroxymethylisoindolinium salts and their condensed derivatives. Among of cyclic products there are representatives with pharmacological activity. In 2008 – the phenomenon of isomerisation of 3a,4-dihydroisoindolinium salts, in 2011 – that Stevens rearrangement of the salts, containing allylic type group along with 4-hydroxybuth-2-ynyl, includes the stages of simultaneously transfer of reaction centre in accepting group and conversion of migrating group, in 2016 – phenomenon of deamination during vacuum distillation of 3-(dialkylamino)-1,4-diarylhex-5-en-1-yns and was worked out the method of preparation of terphenyle and its derivatives.

DAY 2

KEYNOTE FORUM

2nd Global Conference on

Catalysis, Chemical Engineering & Technology

SEPTEMBER 13-15, 2018
ROME, ITALY

CONTENTS

Biography

Q. B. (Rinus) Broxterman (1956) got his PhD degree in 1985 at the University of Groningen (The Netherlands) on an organic chemical topic. He worked for 3 years at an F & F company. From 1988 to April 2017 he worked for DSM in Geleen (NL) in several R&D functions. For more than 10 years he has been Corporate Scientist: responsible for the strategy and quality of the Chemistry &Catalysis competence area. From May 01, 2017, he is CTO of InnoSyn B V. InnoSyn BV is –since May 01, 2107 - an independent chemical process R&D company in Geleen (spin-out of the DSM).

Process design: Un-biased selection and use of catalysis options (chemo-, bio-, photo-) from start to finish (technology platform development to product coming from industrial plant)

Q.B. Broxterman, Ph.D., FRSC

InnoSyn B V, The Netherlands

InnoSyn B V is a chemical process R&D organization located at the Brightlands Chemelot Campus in Geleen, The Netherlands. InnoSyn performs ‘invention’, ‘improvement’ and ‘implementation’ R&D services for its customers and strategic partners.

Organic chemistry combined with several types of catalysis and supported by modern chemical engineering constitutes the technological competences of InnoSyn. Several modern catalysis technology platforms will be described, with elements ranging from technology platform creating at lab scale to development and scale-up to pilot and/or full industrial scale.

InnoSyn has a longstanding track record in (rejuvenation in) bio catalysis and chemo catalysis. Recently, photo catalysis has been added to the catalysis options.

A complex set of factors determine which catalytic solution will be best for any given synthetic challenge. For that reason, InnoSyn finds it important not to be biased in the selection of the type of catalysis.

In some of the examples applying chemo catalysis and photo catalysis, it will be shown that modern chemical engineering /process technology modifications really make the catalysis solutions work.

Bio catalysis

Three biocatalytic technology platforms will be described:

- The development and use of aldolases has already reached full industrial scale for several years (e.g. for manufacturing of statins).
- The exploration, development and use of hydroxylating enzymes and hydratases are of more recent date: recent advances with these platforms will be described. Examples of recent advances of such enzymatic oxy-functionalization are:
    - Direct regioselective hydroxylation of alpha-isophorone and diclofenac
    - Synthesis of 10-hydroxystearic acid by enantio- and regioselective water addition to oleic acid.

Chemo catalysis

A definition of Process Intensification is “Any chemical engineering development that leads to a substantially smaller, cleaner, safer, and more energy-efficient technology”.

When aiming for less hazardous processes that generate less waste, consume less energy, and require less steps and thereby less equipment, catalysis plays an equally significant role to meet these objectives.

At InnoSyn, both (chemo-) catalysis and flow reactors are used to these ends.

Examples of chemo- catalysis platform technologies developed recently:

- Meeting unmet needs in hydrogenation: replacing stoichiometric metal hydride reductions by highly efficient catalytic hydrogenations and asymmetric hydrogenations of notoriously difficult substrate classes;
- Replacing classical biaryl synthesis methods based on pre-functionalized arene coupling partners by single-step, aerobic cross-dehydrogenative arene coupling based on highly active homogeneous Pd catalysts;
- Using 3D printed zig-zag flow reactors for safe oxidations with pure oxygen under high pressure single-phase conditions, exemplified by catalytic aerobic oxidation as a low-cost, low-waste tool for EpoxoneTM production that replaces prior art based on expensive, waste-generating stoichiometric terminal oxidants.

Photo catalysis

Modern LED technology has clear advantages over classical Hg-lamps, and has contributed in reviving photochemistry. This -- combined with falling film reactor set-ups to enable much better irradiation of substrate – constitutes a powerful technology platform in expanding and scaling-up photo chemistry towards industrial manufacturing for fine and specialty chemicals. The combination of features is available from lab up to pilot plant scale, and examples will be discussed.

Audience Take Away:

- Learn several modern (catalytic) technology platforms as they are scale-up and used in chemical industry
- Understand the importance of not being biased in the selection of the type of catalysis to solve a (real life) synthetic problem
- See real life illustrations of the path from developing a technology platform in the laboratory to use on pilot plant and full industrial scale
- Learn examples on how catalysis and chemical engineering concepts are both essential to deliver competitive and scalable novel solutions for synthetic/manufacturing challenges.

CONTENTS

Biography

Christo Boyanov Boyadjiev was born on August 17, 1936, Sliven, Bulgaria. He is a Foreign Member of the Russian Academy of Natural Science – 2008, Professor Emeritus of Bulgarian Academy of Science – 2012, Editor-in-Chief of the "Transactions of Academenergo" (Scientific journal of the Russian Academy of Science), Chairman of the Scientific Council of the International Scientific Centre for Power and Chemical Engineering Problems, Chairman of the Organizing Committee of the Workshop on "Transport Phenomena in Two-Phase Flows"

List of publications (217): http://www.iche.bas.bg/WWW_IChE_EN/LABORATORY_IChE/Process_Systems_Engineering_Laboratory/STAFF_Laboratory/CV_Christo_Boyadjiev/List%20of%20publications.pdf.

MONOGRAPHIES(8): (www.iche.bas.bg/Books_BG.htm).

Awards:

Bulgarian Order of Cyril and Methodius (first class).

Russian Federation Order of Mihailo Lomonosow (National Committee for Public Prizes).

A new approach for modeling of catalytic processes in Industrial column apparatuses

Christo Boyanov Boyadjiev

Institute of Chemical Engineering, Bulgarian Academy of Sciences, Bulgaria

The presented theoretical analysis in the plenary lecture shows, that the mechanics of continua cannot be used to model the gas (liquid)-solid catalytic processes in the column apparatuses, because fluid velocities in the gas (liquid) phase and interphase gas (liquid)-solid boundaries are unknown and cannot be determined. These problems are overcome by replacing the surface (heterogeneous) phase boundary reactions with equivalent volume (homogeneous) reactions, and the unknown phase velocities are replaced by the average velocity of the cross section of the column. This leads to parameters in the models that must be determined by experimental data.

The modeling of the catalytic processes is related with the creation of new type of convection-diffusion and average-concentration models.

The convection-diffusion models permit the qualitative analysis of the processes only, because the velocity distribution in the column is unknown. On this base is possible to be obtained the role of the different effect in the process and to reject those processes, whose relative influence is less than 1%, i.e. to be made process mechanism identification.

The average-concentration models are obtained from the convection-diffusion models, where average velocities and concentrations are introduced. The velocity distributions are introduced by the parameters in the model, which must to be determined experimentally.

The theoretical analysis of the average-concentration models of the catalytic process in the column apparatuses (in the approximations of the mechanics of continua) shows, that the radial non-uniformity of the axial component of the fluid velocity is the reason for the reduction of the efficiency of the processes and the appearance of the experimentally determinable parameters in the models. The plenary lecture shows, that the tangential introduction of the gases (liquids) into the column minimizes the radial non-uniformity of the axial component of the fluid velocity and cancels the values of the experimentally determinable parameters. The only parameters that remain to be determined are the interphase mass transfer coefficients (as volume factors), but they do not depend on the diameter of the column and can be determined by experimental data obtained on a model (small diameter) column.

Audience Take Away:

- The presentation of the plenary lecture will show the audience the possibilities for quantitative description of the catalytic processes in columns in the cases, where the adsorption on the catalyst surface is physical or chemical.
- The presentation of the models of the catalytic processes gives the audience the opportunity to quantify the kinetics of the catalytic processes in the columns and to solve the problems of the optimal process design and control.

CONTENTS

Biography

Dr Cosnier is Research Director at CNRS and head of the Department of Molecular Chemistry at the Grenoble Alpes University (France). His activity is focused on electrochemical biosensors, biofuel cells, electrogenerated polymers, molecular electrochemistry and carbon nanotubes. Dr Cosnier has authored over 340 publications (h-index 56) and 2 books and was the President of the French Group of Bioelectrochemistry (2001-2014). In 2009, he received the Katsumi Niki Prize of the International Society of Electrochemistry and was appointed as Fellow of this Society. In 2013, Dr Cosnier became a member of the Academia Europaea. Finally, he is the recipient of the 2016 China-France Chemistry Award from the Chinese Chemical Society and the Chemical Society of France.

Electroenzymatic catalysis for electrical energy production

Serge Cosnier, Ph.D.
Univ. Grenoble Alpes, CNRS, France

The need for clean methods of producing electricity has stimulated the emergence of new generation of fuel cells. A subcategory of fuel cells, biofuel cells, mainly relies on redox enzymes, which are very efficient and selective biocatalysts that can advantageously replace rare and expensive platinum-based catalysts in classic fuel cell devices. Enzymes provide exceptional specificities towards their substrates, thus enabling the assembly of both the anode and cathode electrodes of a biofuel cell without the need for membranes. These biodevices that convert chemical energy into electrical energy by electro-enzymatic reactions, have attracted considerable attention over the last decade. Recent advances in the design of bioelectrodes based on electrically wired enzymes onto carbon nanotube coatings will be reported. In particular, different strategies for achieving a controlled orientation of laccase or bilirubin oxidase on carbon nanotube-based electrodes for the direct dioxygen reduction will be presented. A new generation of flexible buckypaper electrodes was produced by using linear polynorbornene polymers containing multiple pyrene groups as crosslinker. In addition, the use of bifunctionalized polymers (pyrene and NHS groups) leads to robust buckypapers with the covalent binding of redox groups or enzymes. Moreover, buckypapers based on bilirubin oxidase and FAD-dependent glucose dehydrogenase, were developed for the direct electron transfer and the mediated electron transfer, respectively. The resulting EFC based on the O_2/glucose system, provides the highest volumetric power reported until now, namely 24.07 mW cm^{-3}. The design of hybrid biofuel cells will be also reported. In particular, cubic Pd nanoparticles were synthesized and evaluated for the catalytic oxygen reduction. These nanoparticles were employed for the development of an air-breathing cathode modified by multiwalled carbon nanotubes. The latter was combined with a phenanthrolinequinone/glucose dehydrogenase-based anode to form a complete glucose/O_2 hybrid biofuel cell. Another hybrid system based on hydrogen/air biofuel cell integrating a bioinspired nickel catalyst and a bilirubin oxidase will be described. The biomimetic nickel bis-diphosphine complex immobilized on modified single-wall carbon nanotubes exhibits a reversible electrocatalytic activity for the $H_2/2H^+$ interconversion.

Biomimetic fuel cells involving non-covalently attached network of porphyrins to multi-walled carbon nanotubes will be also described. Pyrene-functionalized Rhodium deuteroporphyrin was used as an anode in the electrocatalytic oxidation of glucose and pyrene-functionalized tetracarboxyphenyl Cobalt porphyrin was used as a cathode in the electrocatalytic reduction of oxygen. The resulting glucose fuel cell led to a maximum power output of 0.9(± 0.10) mW cm-2. Finally, an innovative approach based on the electrical wiring of enzymes in solution by redox glyconanoparticles resulting from the self-assembly of bio-sourced block copolymers will be presented. We demonstrate the self-assembly, characterization and bioelectrocatalysis of redox-active cyclodextrin-coated nanoparticles. The nanoparticles with host-guest functionality are easy to assemble and permit entrapment of hydrophobic redox molecules in aqueous solution. The nanoparticles (diameter: 195 nm) were used as electron shuttles between electrode and bilirubin oxidase providing enhanced current densities for enzymatic O_2 reduction.

Audience Take Away:

- Modification of electrode surfaces for electrocatalysis
- Biocatalysis based on redox organic nanoparticles
- Bioconversion of energy by biofuel cells
- Biomimetic catalysts for O2 reduction and H2 oxidation
- Electrical wiring of enzymes
- The reported strategies for the use of carbon nanotube coatings is relatively easy to exploit for developing electrocatalysis or biocatalysis. The procedures described for the enzyme immobilization and their electrical wiring may be also used by the audience. The concept of biofuel cells may also open new routes for people.
- Of course, other faculty could use to expand their research, for instance the chemical or biochemical functionalization of surfaces may be widely exploited. These concepts could also be used for teaching
- The implanted biofuel cells provide a practical solution to the powering of implanted sensors and medical devices in human body.

Biography

Luis Sánchez Granados born in 1967, he graduated in Chemistry in 1991, obtaining his Ph.D. in 1994 (Chemical Sciences; University of Córdoba). He is Full Professor of Inorganic Chemistry at the University of Córdoba (UCO; Spain). The academic and scientific career has been completed through stages at highly reputed European institutions: CNRS (France); Open University (United Kingdom); Padova University (Italia). His scientific activity is documented by more than 95 papers, 1 patent, chapters to books and over 110 conference communications. This activity is developed in the field of electrochemistry, solid state chemistry, building materials, environmental remediation and photocatalysis, putting special attention to the design of functional materials (oxides, chalcogenides, metals, etc.) in variable forms: micro-nano powders, thin films, 3D arrays. For his scientific activity, he was awarded: Prize of Spanish Royal Society of Chemistry—Novel Research (1998).

ZnO based photocatalysts for enhanced urban air purification

Luis Sánchez Granados, Ph.D.
Universidad de Córdoba, Spain

The elimination of the gaseous pollutants is an environmental issue of huge scientific and social interest. The contamination of urban areas by NOx gases is becoming a severe environmental and human health issue, since many towns worldwide frequently suffer peaks in NOx contamination, far superior to the current legislation's approved values.

Photocatalysis is one of the technologies that could be applied in the remediation of this problem, where TiO_2 and TiO_2-based compounds are more extensively studied as one of the most efficient photocatalytic systems for the oxidative decomposition of NOx (deNOx). In this sense, a broad catalogue of titania based photocatalytic building materials (benchmark products) are known today. Unfortunately, in spite of their excellent performance as photocatalyst, TiO_2 has just been proposed to be classified as suspected of causing cancer when inhaled. This could limit their applications and, therefore, a rapid advance in the study and development of new deNOx photocatalysts is required.

In this work we study the deNOx ability of ZnO based photocatalysts. Even though ZnO, a proved safe compound, is a preferred photocatalyst because its high photosensitivity, mechanical-thermal stability and tunable morphology, only very scarce studies have been recently reported for this application.

Two new deNOx photocatalysts are here presented:

i)ZnAl-CO_3 LDHs. Because of their unique properties and easy preparation, layered double hydroxides (LDHs), also known as hidrotalcite-like materials, have been studied for many potential applications. In the recent years, these compounds have also emerged as an important photocatalyst group. By first time is here studied the application of LDHs to remove NO from air.

ii)ZnO/SiO_2 composites prepared by a simple methodology using of rice husk ash (RHA) as photocatalyst support, a strategy successfully employed in the preparation of metals and metal oxides (photo) catalysts.

The physico-chemical characterization and photocatalytic activity of different ZnO based compounds are presented. Remarkably, the studied compounds exhibit high efficiency and selectivity towards the photocatalytic elimination of NO from air.

Audience Take Away:

- The use of waste´s valorization as tool to enhance the photocatalyst activity
- The use of cost-effective and large-scale synthetic procedures to obtaining new photocatalysts.
- The preparation of sustainable photocatalysts with potential practical use to combat the polluted atmosphere in urban environments.

CONTENTS

Tuning zeolitic parameters for the trapping and elimination of pollutants and toxic gases – application in automotive cold-start and nuclear safety

Bruno Azambre, Ph.D.

University of Lorraine, France

Biography

Bruno Azambre is 45 years old and is Associate Professor (Hab.) at University of Lorraine – Institut Jean Barriol (France). After a PhD thesis in Metz devoted to the catalytic/sorption properties of functionalized carbons (2000), he worked as post-doc at University of Reading (UK) on inorganic nanotubes. When in 2003 he became a permanent lecturer, he examined the reactivity of pollutants with sorbents/catalysts in numerous fields such as automotive depollution, AOP's, nuclear safety and others. His works are devoted to the design, surface characterization, testing of reactive materials (zeolites, rare-earth oxides, carbons, mesoporous materials) and the elucidation of complex mechanisms by in situ/operando spectroscopies. He is co-author of about 60 publications and 100 communications.

The development of new trapping and abatement strategies is key in order to avoid the dissemination of harmful pollutants and toxic substances into the environment. By comparison with physisorption-related processes, irreversible trapping generally involves chemisorption or catalytic reactions of the targeted molecules on the active sites of specifically-designed materials. Well-known applications include for instance the trapping of NOx and SOx or the catalytic elimination of diesel soot in DPF. In these last years, new applications are emerging. A key target to reduce current hydrocarbon (HC) emissions from automotive exhausts is to improve their abatement under cold-start conditions, which mostly arise during the first two minutes of the driving cycle. One of the most promising after-treatment technology is to trap the HC at low temperatures on a sorbent, typically a zeolitic material, which can be combined with an oxidation or a deNOx catalyst, so that the desorbing HC can be easily burnt at higher temperatures or alternatively reduce nitrogen oxides. In that respect, the zeolitic material has to be not selective to the type of HC (i.e. propene, toluene and decane) and the HC desorption temperature has to be high enough to match with the light-off temperature of the oxidation or DeNOx catalyst. Another emerging application for zeolitic materials is their use as iodine trap in the context of a severe nuclear accident (Fukushima-like). In that respect, it has to be ensured that no radioactive iodine could be released from the filter under dynamic flowing conditions over a long period. Stable trapping could in principle be obtained using specifically-tailored silver zeolites thanks to the formation of AgI precipitates involving the catalytic transformation of CH_3I and I_2 on silver sites. In both applications, the zeolitic filter has to withstand the presence of inhibitors (H_2O, COx, NOx…) and maintain its properties over a wide range of temperatures.

In this presentation, we will see how it is possible to finely tune the zeolitic parameters, such as the pore size and connectivity, the Si/Al ratio, the nature and content of compensating cations in order to meet the above-mentioned requirements in both applications. A screening of several zeolitic sorbents will be presented thanks to a quantitative evaluation of multiple breakthrough curves, TPD and TPSR data. Characterization of the materials before and after test, as well as the use of in situ diffuse reflectance spectroscopies (DRIFTS and DRS-UV-Vis) will provide important insight on the nature of active sites and the complex network of reactions associated with the storage and decomposition of trapped molecules under representative conditions.

CONTENTS

Audience Take Away:

- From an application viewpoint, the audience will learn important aspects relevant to: (i) the removal of unburnt hydrocarbons emitted in the cold-start phase of light vehicles ; (ii) the trapping of radioactive iodine in the context of a nuclear accident. From a methodological viewpoint, this talk will give insights into the tailored design an adsorbent/catalyst for a targeted application and the unravelling of surface mechanisms by after-test characterization and in situ spectroscopies.
- This presentation should help to unravel the effects of the zeolitic framework, the nature of exchanged metal ion and the preparation method on the trapping of pollutants when present alone or in complex mixtures. General guidelines will be provided to understand the factors playing a role on the adsorption selectivity and/or catalytic decomposition to by-products, pore blocage etc... A list of the more appropriate for the above-listed applications will be given on a rational basis. Links to other relevant processes, such as catalytic oxidation, NOx-SCR for automotive cold-start and methanol to olefins (MTO) for CH3I trapping will be given.

DAY 2

SPEAKERS

2nd Global Conference on

Catalysis, Chemical Engineering & Technology

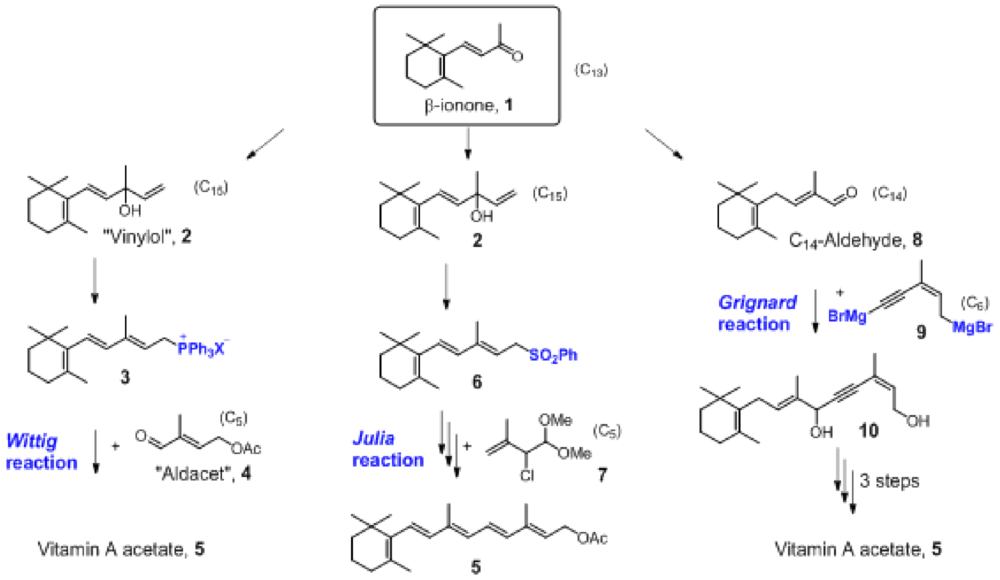
SEPTEMBER 13-15, 2018
ROME, ITALY

CONTENTS

Catalytic routes to Vitamin A Acetate

Jan Schütz*, W. Bonrath, C. Eggertswyler, J. Medlock, T. Netscher, B. Wüstenberg
Research and Development, DSM Nutritional Products, CH-4002 Basel, Switzerland

Vitamin A is a lipid-soluble vitamin, which is essential for the vision process, growth, and cell functions. Dietary deficiency symptoms are e.g. reduced immune response and growth retardation in animals and night blindness in humans. On an industrial scale vitamin A is produced by chemical synthesis based on β-ionone (1). In 100 years of vitamin research only three vitamin A processes have been industrialized. All production processes apply stoichiometric reactions with activated reagents (Wittig: 3+4→5; Julia: 6+7→5; Grignard: 8+9→10) which generate equimolar amounts of by-products. [1-3] A direct catalytic route to vitamin A acetate (5) (avoiding protecting group chemistry) does not exist so far.



Several catalytic coupling reactions were investigated using compounds based on β-ionone (1) as preferred starting material for the cyclohexene moiety of vitamin A acetate, in combination with a variety of other smaller (< C6) building blocks. With these methods, the use of stoichiometric coupling conditions resulting in the formation of equimolar amounts of waste streams can be avoided.

Audience Take Away:

- Methods how to substitute stoichiometric reactions by catalytic ones
- Get to know highly optimized syntheses of complex fine chemicals
- Step by step improvement of a synthesis route by introducing catalytic reaction steps
- Get insight into process research in fine chemical industry

Biography

Jan Schütz studied in his diploma thesis at Stanford University in the group of Prof. R. Waymouth the synthesis and self-assembly of micellar block copolymers and their use as novel catalytic media. In his PhD thesis he investigated the synthesis and application of N-heterocyclic carbene metal complexes in catalysis in the group of Prof. W. A. Herrmnann at the Technical University of Munich. During his PostDoc at DSM Nutritional Products in the group of Dr. W. Bonrath he studied solid bases in aldol condensations to intermediates of vitamins. Since 2006 he is lab head at DSM Nutritional Products, Process Research in catalysis and organic synthesis of vitamins, nutraceuticals, and aroma ingredients. Special focus is on steroid chemistry, such as vitamin D3 and derivatives and in heterogeneous catalysis with focus on gas phase reactions.

Plasma modification of α-Fe_2O_3 supported nanomaterials for photocatalytic and photoelectrochemical applications

Alberto Gasparotto[1]*, Ph.D., Giorgio Carraro[1], Ph.D., Chiara Maccato[1], Ph.D., Davide Barreca[2], Ph.D.
[1]Department of Chemical Sciences, Padova University and INSTM, 35131 Padova, Italy
[2]CNR-ICMATE and INSTM, Department of Chemical Sciences, Padova University, 35131 Padova, Italy

Hematite (α-Fe_2O_3), the most stable phase of iron(III) oxide, is an appealing active material for various photocatalytic and photoelectrochemical applications concerning sustainable energy generation and environmental remediation. In fact, beyond its favorable catalytic and electronic properties, as well as its band gap of 2.1 eV which allows absorption of Vis photons, this semiconductor exhibits an appreciable chemical stability and is cheap, abundant and nontoxic. Nevertheless, various hematite drawbacks, such as the relatively low absorption coefficient, short lifetime of photogenerated charge carriers (e-/h+), small hole diffusion length and slow reaction kinetics, have prevented up to now the achievement of satisfactory efficiencies.

An amenable strategy to circumvent these drawbacks and obtain improved performances, involves functionalization of α-Fe_2O_3 by doping or surface modification with suitable nanoparticles or (ultra)thin layers. In this way, additive or synergistic effects arising from the combination of two or more material components come into play. These effects might include, among others, an increased light harvesting, a higher surface reactivity, a reduced recombination of photogenerated e-/h+pairs and their more effective exploitation in the target chemical processes.

In order to fully exploit the advantages originating from α-Fe_2O_3 modification, a proper design of the final material is imperative to control its morphology, surface area, defect content and interface quality, all these characteristics being directly interrelated with the ultimate functional properties.

In the field of inorganic nanosystems, plasma-assisted routes such as sputtering and plasma enhanced-chemical vapor deposition (PE-CVD) offer a high control over topological, structural and compositional material features, impacting, in turn, a broad variety of technological applications.

In this contribution, attention will be focused on selected case studies demonstrating the high potential of plasma processing in the tailored fabrication of Fe_2O_3-based functional nanostructures. Representative examples will include:

i) the synthesis of Pt/α-Fe_2O_3 nanocomposites by a hybrid synthetic route, consisting in the PE-CVD of iron(III) oxide followed by platinum radiofrequency (RF-) sputtering and eventual annealing in air. Material characteristics such as Pt oxidation state and hematite nano-organization could be finely tuned as a function of the adopted processing conditions and strongly affected the system performances in sunlight-assisted photoelectrochemical water splitting;

ii) α-Fe_2O_3-TiO_2-Au composites, fabricated by a three-step plasma-assisted strategy, and tested in the solar-driven H_2 generation via photoreforming of ethanol aqueous solutions. Compared to bare hematite, Fe_2O_3-TiO_2-Au photocatalysts displayed an improved functional behavior, rationalized in terms of an enhanced interfacial charge carrier separation and an improved light harvesting;

iii) supported nanocomposites, prepared by a sequential PE-CVD/RF-sputtering approach and successfully tested in gas-phase photocatalytic abatement of NOx (NO + NO_2) driven by solar illumination. In this case, a good interfacial quality and an intimate Fe_2O_3/TiO_2 contact was achieved, of key importance to exploit the chemical and electronic coupling between the two oxides. As a consequence, the obtained composites featured a remarkable activity in NOx removal, candidating them as valuable photocatalysts for the abatement of harmful atmospheric pollutants.

Audience Take Away:

- Knowledge about the importance of surface modification to achieve improved functional performances
- Highlights on the flexibility and unusual properties offered by cold plasma technologies in the processing of nanoscale materials
- Novel concepts concerning the tailored design of nanostructured supported catalysts for photocatalysis and photoelectrochemical applications

CONTENTS

Biography

Alberto Gasparotto graduated in Chemistry in 2002 and received his PhD in Chemical Sciences in 2006. Since 2016 he is Professor of General and Inorganic Chemistry at Padova University, Italy. His research is mainly devoted to the study of structure-property relationships in inorganic and hybrid nanosystems developed by advanced and unconventional techniques typically involving Chemical Vapor Deposition (CVD), plasma-CVD and plasma sputtering. For his scientific activity, documented by more than 180 scientific papers, he has been awarded, among others, the Prize for the Best PhD Thesis in Inorganic Chemistry by the Italian Chemical Society (2006), the "Eni Italgas Prize for Energy and Environment - Debut in Research" (2007), the "Prize for extra-ordinary innovation: answer to the challenges of the planet" (2008), and the Sapio Prize for Italian Research (2009).

CONTENTS

In-situ and Operando soft X-ray absorption spectroscopy on water oxidation catalysts

Kathrin Maria Aziz-Lange
Helmholtz Zentrum Berlin für Materialien und Energie & Bielefeld University, Germany

Hydrogen gas (H_2) is currently being pursued as an alternative energy carrier to replace fossil fuels. Solar-driven splitting of water into O_2 and H_2 is one of the intensively discussed approaches to obtain hydrogen. For a knowledge driven development and optimization of stable low-cost photocatalytic systems a detailed understanding of the structure-function correlation of these materials is required. Synchrotron-based operando soft X-ray spectroscopy can provide important insights into the electronic structure during the catalytic function. However, bridging the pressure gap between the experimentally necessary vacuum conditions and the operando conditions involving electrolyte solution, applied voltage or light irradiation is challenging. Here, a recently developed soft X-ray transmission cell for in-situ and operando X-ray absorption spectroscopy studies at the synchrotron facility BESSYII will be presented together with recent studies on catalytic systems. Using the example of a MnOx water oxidation catalyst the power of transition metal L-edge spectroscopy will be presented, allowing to reveal how contributions from different material structures and oxidation state species change during the activation process of the catalyst. The XAS results show that the freshly prepared film at OCP contains a dominant contribution of MnO_2 (~75 %) and a contribution from a birnessite-like material (~25%). No or only neglectable percentage of MnO, Mn_3O_4 or Mn_2O_3-like Mn species were found in the freshly prepared sample. After 51 min of in situ activation at 1.2 V vs NHE at pH 7.0, the birnessite-contribution increased to 75% in the spectrum. As another example oxygen K-edge measurement will be shown, that were applied to investigate the role of oxygen during the oxygen evolution reaction (OER) in an electrodeposited Ni-Fe(OxHy) electrocatalyst. For the first time, we tracked here the spectral changes in a dynamic fashion in the soft X-ray regimes during cyclic voltammetry (in situ CV-XAS) to obtain a fine-tuned resolution of the potential-related changes. At operando conditions we observed the formation of a pre-peak feature at the O K-edge which we correlated to the formation of an electron deficient oxygen site.

Audience Take Away:

- The audience will learn, how operando XAS works and how it can be applied for elucidating the electronic structure of catalysts.
- The here presented method and cells are available for all researchers who apply for beamtime at the BESSYII synchrotron facility
- The presented technique can help the authors for developing a structure-function-correlation for their materials

Biography

Kathrin Maria Aziz-Lange, whose research straddles the fields of synchrotron x-ray spectroscopy and energy materials, is a Junior Professor at Bielefeld University and Helmholtz-Zentrum Berlin für Materialien und Energie. She became involved with synchrotron radiation in 2009 during her thesis work on high-resolution XES measurements on the hydrogen bond network of liquid water, that was award with the Wilhelm-Ostwald Nachwuchs prize by the Gesellschaft Deutscher Chemiker. Following a postdoc at the Max-Born Institute Berlin and a research stay at the École Polytechnique Fédérale Lausanne on ultrafast liquid spectroscopy she returned to HZB. Since 2016 she is leading there and in Bielefeld the Helmholtz Young Investigator group Operando Characterization of Solar Fuel Materials focusing on the development of synchrotron based in-situ and operando characterization techniques to elucidate the electronic structure of energy conversion materials during function.

Deactivation/regeneration cycles of Rh/C and Ru/C for the valorization of chloromethanes by hydrodechlorination

María Martín Martínez*, Ph.D., Rodriguez J.J., Ph.D., Gómez-Sainero, L.M., Ph.D.
Universidad Autónoma de Madrid, Spain

Chloromethanes (CMs) are chlorinated volatile organic compounds, with high toxicity and carcinogenic character, which contribute to global warming, ozone layer depletion and photochemical smog. There exist several technologies available for the abatement of CMs from residual streams. Nevertheless, the valorization of these compounds, aiming their transformation into valuable hydrocarbons, is a very interesting alternative to the traditional treatments of CMs. In previous studies, the gas phase hydrodechlorination (HDC) of dichloromethane (DCM) and chloroform (TCM) with Pd/C, Pt/C, Rh/C and Ru/C catalysts was investigated, finding important differences in their activity, selectivity and stability. While Pt/C showed an exceptional stability, Pd/C exhibited the highest CM conversion and selectivity to hydrocarbons with more than one carbon atom (C^{1+}). Rh/C and Ru/C also showed high selectivities to C^{1+} and olefins, which constitute very important industry feedstocks. Nevertheless, they suffered a severe deactivation with time on stream. In this work, the behavior of Rh/C and Ru/C in the HDC of DCM and TCM is studied, analyzing the relationship between their chemical and physical properties and their activity. In addition, a catalyst regeneration treatment is proposed. Rh/C and Ru/C (1 wt.%) were synthesized by incipient wetness impregnation of a commercial activated carbon, and activated by reduction with H_2 at 250 °C. Their catalytic activity was determined in hydrodechlorination experiments carried out at atmospheric pressure, using an inlet CM concentration of 1000 ppm, a molar H_2/CM of 100, a temperature of 250 °C and a space-time of 1,7 kg h mol^{-1}. The catalysts were characterized before and after the hydrodechlorination reaction by adsorption-desorption of N_2 at -196 °C, CO chemisorption, X-ray photoelectron spectroscopy, X-ray diffraction and thermogravimetric analysis. Catalysts deactivation was attributed to the adsorption of chlorinated compounds to the active sites, the formation of carbonaceous deposits blocking the porous structure and metal sintering. Catalysts regeneration by oxidizing treatment at 250 °C led to the complete recover of initial activity, favoring the selectivity to olefins.

Audience Take Away:

- Chloromethanes are very dangerous products present in several industrial streams.
- Catalytic hydrodechlorination is a promising technology for the abatement of chlorinated organic compounds, such as chloromethanes.
- Catalytic hydrodechlorination of chlorinated organic compounds can be used for the production of valuable hydrocarbons, like C1+ and olefins, which could serve as feedstocks for the petrochemical industry.
- Catalysts deactivation is one of the main problems of catalytic hydrodechlorination with Rh/C and Ru/C. But catalysts regeneration by oxidizing treatment permits to work in short cycles of deactivation-regeneration, favoring the production of valuable olefins.

Biography

Graduated in Chemistry, in 2014 she received her Ph.D. in Chemical Engineering from Universidad Autónoma de Madrid (UAM, Spain). In 2012, she works at University of St. Andrews (Scotland, UK) for 4 months, to complete her PhD investigation. During 2015 and 2016, she was a postdoctoral researcher at the Laboratory of Separation and Reaction Engineering-Laboratory of Catalysis and Materials (Associate Laboratory LSRE-LCM), in Portugal. Since 2017, she is developing her scientific career at UAM (Spain). Her research interests are related to the environmental engineering field, mainly focused on the treatment of industrial water and gas streams.

A study on simultaneous reduction of CH_4 and NOx of NGOC/de-NOx catalysts for CNG buses

Choong Kil Seo, Ph.D.
Howon University, Republic of Korea

Natural gas is a clean fuel that discharges almost no substance contaminating the air. It has mainly been used as the primary fuel source for the CNG (Compressed Natural Gas) bus. Application of natural gas, with many advantages as a fuel, is anticipated to spread more widely, thanks to the rich deposit of shale gas and innovative drilling technologies and its stabilized price. However, CH_4 is one of the culprits of greenhouse effect and its impact is 23 times greater than CO_2 of the same mass. As of now, laws require the city bus to use CNG fuel, the primary content of which is CH_4. A currently commercialized after-treatment system for reducing CH_4 and NOx for CNG buses is run by a theoretical air-fuel ratio and uses a three-way catalyst. Operation in a theoretical air-fuel ratio involves deterioration of fuel-efficiency and more emission of CO_2, while the after-treatment system of a lean air-fuel ratio type, increases in cost and difficulties in installation, due to the size of the catalyst unit. This study targets developing a NGOC/LNT+NGOC/SCR combined unit for a simple “one canning two brick system” that can simultaneously reduce the emission of CH_4 and NOx for the CNG bus, in response to post Euro 6 emission regulation, which will be challenging and make this study more meaningful. This study is mainly focused on identifying the loading amount of precious metals, additive catalysts, loading amount of washcoat and stirring time and types of substrates, related with improvement of de-CH_4/NOx performance.

Audience Take Away:

- In this study, the following results were obtained through the the loading amount of precious metals, additive catalysts, loading amount of washcoat and stirring time and types of substrates, related with improvement of de-CH_4/NOx performance.
- In case of a higher loading amount of 6Pd, the Pd dispersion decreased and the catalyst’s reaction velocity deteriorated due to the increased size of particles, which eventually declined the harmful gas reducing performance. In order to improve the stable substance, CH_4 reducing performance, it was estimated to adopt the 3Pd loading amount, by taking into consideration the de-CH_4 performance and the economic feasibility of precious metal Pd.
- CH_4 conversion rate of 3Ni loaded NGOC catalyst generally showed a better performance in CH_4 reduction, starting to oxidize at 350ºC to 400ºC. Ni is an alkaline, toxic oxide so easily activated when mixed with CH_4, chemically stabilized. In reducing NO at a low temperature, the appropriate amount was 5Cr, this was because Cr is a strong acid oxide so readily reacts to stabilized metal oxides as well as oxidization and reduction of between NO and CO particles.
- The NGOC catalyst loaded with an appropriate amount of 124g/L washcoat began to oxidize at 375ºC and showed the highest de-CH_4 removing performance as the temperature reached 500ºC and LOT50. In addition, with the economic feasibility of catalysts considered, an appropriate amount of catalyst washcoat loading was estimated to be 124g/L.
- NGOC/LNT catalysts of ceramic substrates started to oxide CH_4 at 325ºC to reach 550ºC and LOT 50; it showed a de-CH_4 removal performance, about 20% higher than NGOC/LNT catalysts of metal substrates. This was the result of the washcoats loaded in metal substrates were concentrated highly on one side, compared with the ceramic substrates with a honeycomb shape, and their dispersion was deteriorated.

Biography

Chung-Kil Seo is an associate professor at the Department of Automotive Engineering at Howon University in Gunsan, Jeollabuk-do, Republic of South Korea. The major is combustion and post-exhaust treatment engineering, renewable energy. In particular, I have devoted to catalytic research and development, which is an exhaust gas abatement device for diesel vehicles, and have contributed to practical use of de-NOx catalysts (Lean NOx Tran & Selective Catalytic Reduction). I received a Ph. D. degree in the Department of Mechanical Engineering from Chonnam National University at Gwangju city in February 2012. I have been working on the environmentally friendly diesel hybrid research center of Korea Automotive Technology Institute (KATECH) under the Ministry of Tread, Industry and Energy, and mainly developed the catalysis for vehicles and sensors.

CONTENTS

Infrared spectroscopy for ranking zeolite acidity: The VTIR method

Montserrat Rodriguez Delgado*, Ph.D., C. Otero Arean, Ph.D.
University of the Balearic Islands, Spain

Bronsted-acid zeolites, which contain the structural unit [Si(OH)Al], are currently used as catalysts in a wide range of technological processes, spanning from the petrochemical industry to biomass upgrade and the production of fine chemicals, to name only a few examples. For many of the chemical processes involved in those applications appropriate acid strength is a key factor determining catalytic performance, and hence the convenience to have a reliable method for evaluating relative Bronsted acidity. On account of its easy implementation, IR spectroscopy (at a fixed low temperature) of an adsorbed weak base, which interacts with the zeolite OH groups by hydrogen bonding, is a very frequently used instrumental technique to rank zeolite acidity, and carbon monoxide is the probe molecule of choice. The H-bonded species ZO-H···CO (where Z stands for the zeolite framework) can easily be monitored by IR spectroscopy, as hydrogen bonding brings about a characteristic red shift, $\Delta\nu$OH, of the O-H stretching frequency. The magnitude of such a shift is frequently used to rank Brønsted acidity of protonic zeolites. Nonetheless, the enthalpy change ΔH0 involved in the hydrogen-bonding interaction should be a more reliable indicator. In fact $\Delta\nu$OH and ΔH0 are often found to correlate among themselves; but that is not always the case. We report herein on the application of variable-temperature IR (VTIR) spectroscopy to determine, simultaneously, $\Delta\nu$OH and ΔH0; and revise recent experimental results showing how the usual practice of ranking Brønsted acid strength of zeolites by the corresponding O-H frequency shift probed by an adsorbed weak base can sometimes be misleading.

Audience Take Away:

- Awareness of possible pitfalls of using IR spectroscopy at a fixed temperature when ranking acidity of zeolites by using a weak base probe molecule.
- Knowledge about the advantage of a recently developed technique, termed VTIR spectroscopy, that facilitates simultaneous determination of $\Delta\nu$OH and ΔH0, when using an infrared probe molecule.
- An overview of recent experimental work showing some examples where $\Delta\nu$OH and ΔH0 are not directly correlated among themselves.

Biography

Montserrat Rodriguez Delgado obtained her BSc and PhD degrees in Chemistry at the University of the Balearic Islands (Spain), and she carried out pre-doctoral research at the University of Caen (France) and postdoctoral research at the Universities of Turin (Italy) and Madrid (Complutense). Currently, she is Senior Lecturer of Inorganic Chemistry and Materials Science at the University of the Balearic Islands; where her main research interests are in several areas of surface science (with a focus on phenomena occurring at the solid–gas interface), zeolites, and nanostructured materials for advanced environmental and technological applications.

Cyclodextrins as a versatile tool for Organometallic catalytic processes

Sébastien Tilloy
University of Artois, CNRS, UCCS, France

Green chemistry is a movement whose goal is to develop more environmentally friendly methods for the chemical industry. Use of (i) catalytic reagents and (ii) replacement of organic solvents are two of the main points of this movement. In this context, we proposed the use of cyclodextrins (CDs) family (i) as ligands for transition metals and (ii) as solvents for aqueous organometallic catalytic processes.

CD as ligands: In these processes, the catalyst is generally immobilized in water by water-soluble ligands such as phosphanes. These phosphanes are obtained by attaching water-solubilizing groups to known hydrophobic phosphanes. Among these groups, the CDs family is a very interesting class of hydrophilic block since phosphanes based on a CD skeleton can combine the molecular recognition and catalytic properties in the same entity. In this context, we reported the synthesis of new water-soluble cyclodextrin-phosphanes (CD-P). Organometallic complexes formed by these CD-phosphanes associated to a rhodium precursor are efficient in hydroformylation reaction. It is important to underline that the activity and selectivity of hydroformylation reaction can be tuned by the nature of the guest.

CD as solvents: Recently, a new family of solvents, so-called low melting mixtures (LMMs), have emerged in the current literature. In this context, LMMs based on N, N'-dimethylurea (DMU) and various β-cyclodextrins (CD) have been prepared for organometallic catalysis applications. These mixtures are easily obtained by simple association of CD and DMU around 90°C. These solvents are based on commercially available compounds and easily handled. These LMMs were evaluated as solvent in rhodium-catalyzed hydroformylation reaction and in palladium-catalyzed cleavage of allylcarbonates (Tsuji-Trost reaction). This solvent offered a simple handling and a protection of the catalytic species confined in the solvent at the solid state.

Audience Take Away:

- This oral communication will deal with (i) Green Chemistry, (ii) Supramolecular Chemistry and (iii) Organometallic Catalysis. The audience will acquire knowledge and skills in these fields.
- This oral could provide solutions to synthetize water-soluble organometallic catalysts and to use supramolecular receptor (cyclodextrin) to functionalize numerous kinds of substrates.

Biography

Sébastien Tilloy was born in 1972 (France). He received his Ph.D degree in 1998 from the University of Artois. In 2000, he became Associate Professor at the University of Artois where he completed his Habilitation in 2004. In 2005, he moved to University of Amsterdam (Netherlands) to work with Pr. Leeuwen and Pr. Reek. In 2006, he was promoted Full Professor. His research interests are centred on the cyclodextrins and on their supramolecular implications in the field of organometallic catalysis. He is the author of 85 international publications (h-index 30), 4 patents, 3 chapters and more than 80 oral/poster presentations.

A near ambient pressure X-ray photoelectron spectroscopy study on Platinum nanoparticles supported on Zr-based metal organic frameworks

Reza Vakili[1*], Ph.D., Xiaolei Fan[1], Ph.D., Alex Walton[2], Ph.D.
[1]School of Chemical Engineering and Analytical Science, The University of Manchester, Manchester, M13 9PL, United Kingdom
[2]School of Chemistry, The University of Manchester, Manchester, M13 9PL, United Kingdom

The first near ambient pressure (NAP)-XPS study of CO oxidation over Pt nanoparticles (NPs) incorporated into Zr-based UiO (UiO for Universitetet i Oslo) MOFs was carried out. For this Purpose, the MOF-based Catalysts were prepared by wetness impregnation (WI-PtNPs@UiO-67) and linker design (LD-PtNPs@UiO-67) methods along with PtNPs@ZrO_2 as the control catalyst. Firstly, the as-synthesized catalysts were reduced in situ prior to the operando XPS analysis. The existence of Pt(II) species was proved in UiO-67 by observing Pt 4f core level peaks at a high binding energy of 72.6±0.1 eV. After the reduction, the higher BE components disappear, leaving only the metallic Pt 4f doublet, confirming the formation of Pt NPs. To understand the chemical state of Pt NPs in UiO-67 during catalytic turnover, we analyzed the Pt 4f region using operando NAP-XPS in the temperature-programmed measurements (100–260 °C) with reference to PtNPs@ZrO_2 catalyst. Pt 4f peaks only show one chemical species present at all temperatures, but the core level BE shifts change as a function of reaction temperature, i.e. Pt 4f peak from 71.8 eV at $T < 200$ °C to 71.2 eV at $T > 200$ °C. As this higher BE state of 71.8 eV was not observed after in situ reduction of the catalysts and only once the CO/O_2 mixture was introduced, we attribute it to the surface saturation of Pt NPs with adsorbed CO. In general, the quantitative analysis of Pt 4f data from the operando NAP-XPS experiments shows that the surface chemistry of the Pt active phase in the two PtNPs@UiO-67 catalysts is the same, comparable to that of PtNPs@ZrO_2. The observed difference in the catalytic activity can be attributed to the particle sizes of Pt NPs, as well as the dispersion of active phase in the support, which are different in the three catalysts.

Audience Take Away:

- The potentials of metal organic frameworks (MOFs) as catalytic supports are discussed
- Different synthesis methods to prepare MOF-based catalysts are introduced
- The results of NAP-XPS study of CO oxidation over Pt nanoparticles (NPs) incorporated into Zr-based are presented
- The superiority of MOF-based catalysts over commercial one (Pt/ZrO_2) is shown.

Biography

Reza vakili got his MSc degree in Chemical Engineering from Shiraz University, Iran. During his MSc studies, he focused on simulation and optimization of different chemical reactors, including fixed-bed and fluidized-bed reactors. Currently, Reza is a PhD student in Chemical Engineering at the University of Manchester. His PhD research project focuses on MOFs for heterogeneous catalysis.

CONTENTS

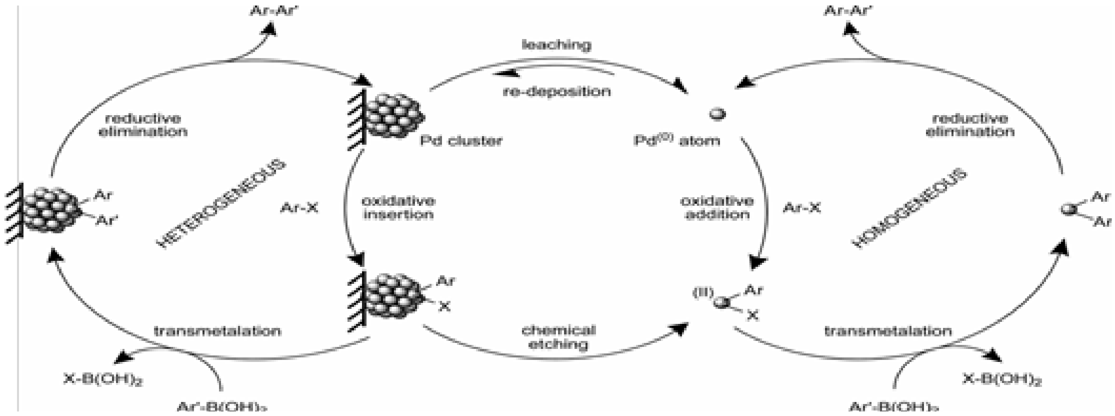
Innovative flow reactor to study the nature of active species in suzuki- miyaura reaction of iodoacetophenone with phenylboronic acid in ethanol

Amine Bourouina*, Valérie Meille, Claude De Bellefon
LGPC (UMR5285 CNRS/CPE Lyon/UCBL), VILLEURBANNE cedex, 69616, France

The Suzuki-Miyaura reaction (SMR) and more generally the carbon-carbon (C-C) coupling reactions catalyzed by Pd have been the subject of numerous and prolific research in organic chemistry catalysis. Indeed, it was crowned by the awarding of the Nobel Prize in Chemistry to Richard Heck, Ei- ichi Negishi and Akira Suzuki in 2010.

Several studies have been conducted to determine the nature and origin of the active species in the mechanism of this reaction when using a heterogeneous catalyst based on palladium but, this question remains open. Some authors postulating a purely heterogeneous mechanism and others a homogeneous mechanism (Fig. 1) in which a catalytically active molecular complex is formed from the palladium nanoparticle. Moreover, the understanding of this mechanism will help to revolutionize the implementation of the SMR reaction which is widely used industrially.

Figure 1. Proposed Mechanism for the supported PdNP-Catalyzed Suzuki Cross-Coupling



Involving Both Homogeneous and Heterogeneous Pathways

An innovative flow reactor (Fig. 2) was used for the determination of the nature of the mechanism. The idea is to build a column filled with a heterogeneous catalytic precursor, and add a tubular reactor just after the column. The catalytic solid is only in the column. So, if the mechanism is heterogeneous, the conversion at the outlet of the tubular reactor must be equal to that at the outlet of the column. ICP-MS is used to estimate the amount of leached palladium.

The results showed a large homogeneous contribution in the tubular reactor (Fig. 3) which confirms the formation of homogeneous catalytic species from supported Pd. Modeling on MATLAB©,using two different homogeneous and heterogeneous models has permitted to demonstrate that the catalytic activity in the tube is equal to that in the column, and that only the leached Pd is catalytic (no or negligible heterogeneous contribution in the column).

ICP-MS analysis has shown that a very small amount of palladium (0.1ppm) can catalyze the Suzuki reaction under mild conditions (T= 60 ° C). This amount of Pd corresponds to a TOF ≥ 300,000 h-1 in the tubular reactor.

In this work an innovative continuous reactor was used to verify the nature of the active species that catalyzes the Suzuki reaction of iodoacetophenone with phenylboronic acid, using three commercial catalysts known in the literature to have a heterogeneous mechanism. The obtained results demonstrate that these heterogeneous precursors of Pd are in fact a production sources of highly active species in a homogeneous medium that catalyze the SMR reaction of iodoacetophenone without the catalytic contribution of palladium supported on the solid. Albeit this demonstration is only valid for the reagents used, i.e. iodoacetophenone, future work is devoted to extend it by studying other reagents based on bromides and aryl chlorides which are less active than iodo-aryls.

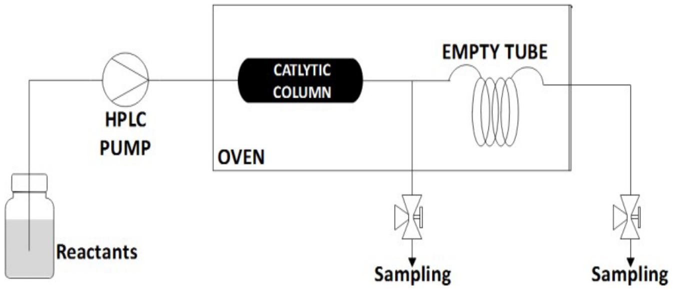


Figure2: Experimental devices used

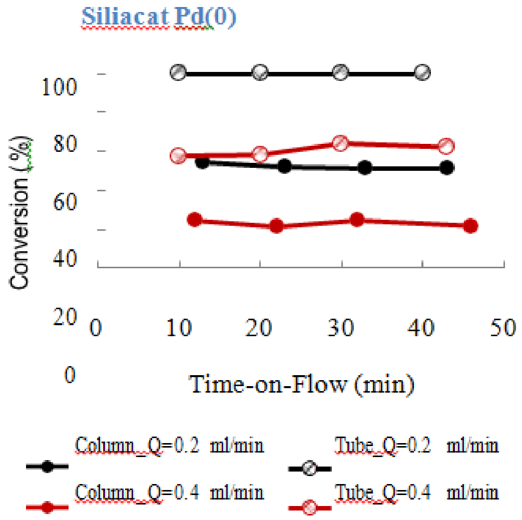


Figure 3: Variation of the column output conversion and tube output. C_A= 0.025 mol/l, C_B=0.03 mol/l, C_{MeONa}=0.038 mol/l, T_{bain}=60°C, Vtube=2.14 ml. Columns: Siliacat_Pd(0) (V_1=0.42 ml, m_{Pd}=8.73 mg), Strem_Pd(0) (V2=0.42 ml, m_{Pd}= 15mg), Siliacat_Pd(II)_DPP (V3=0.02ml, m_{Pd}=0.6mg).

Table 1: Conversions & Pd leaching for 3 catalysts in the SMR coupling of iodoacetophenone and phenylboronic acid. Conditions: see Figure3.

Q (ml/min)	Catalyst	Column (%)	Tube (%)	Pd leach. (ppm)
0.2	Siliacat Pd(0)	50	100	0.12
0.4	Strem Pd(0)	24	56	0.1
1	Siliacat Pd(II) DPP	37	75	0.53

Audience Take Away:

- This work provides a new and simple tool that can be used in flow chemistry to study the homogeneous vs heterogeneous nature of the catalytic species. Albeit it the demonstration is made here for a very restricted range of reagents, we believe that such a simple set-up can be used by a large number of research teams, for many different reactions, to help understanding the nature of catalytic species.

Biography

Amine Bourouina is a 2nd year Ph.D Student at the University Claude Bernard Lyon1 in the field of chemical engineering. His Ph.D thesis is about the study of Suzuki-Miyaura reaction using innovative reactors. He has got two masters in the chemical engineering field (Process Engineering, Refining Oil and Petrochemical). His main research interest covers Reactor modeling – homogeneous & heterogeneous catalysis – flow-chemistry – and kinetic study. Amine has participated in national and international meetings (SFGP, CAFC11 and ICLyon).

Cerium based metal organic frameworks for catalytic CO_2 conversion

Michalina Stawowy*, M.Sc., Janusz Trawczyński, Agata Łamacz, Ph.D.
Department of Fuel Chemistry and Technology, Wrocław University of Science and Technology, Gdańska 7/9, 50-344 Wrocław, Poland

The atmospheric concentration of carbon dioxide has been rising extensively since the Industrial Revolution and has now reached dangerous levels, contributing to climate change. Direct transformation of abundant CO_2 to valuable chemicals and fuels is currently of great importance from the viewpoints of environmental and green chemistry. Utilization of CO_2 as feedstock for methanol synthesis is one of the possibilities. Metal-organic frameworks (MOFs) have recently gained attention as potential catalysts in many reactions. Owing to crystalline nature, chemical tunability, remarkably high surface area and regular pore structure, MOF materials combine some of the best features of homogeneous and heterogeneous catalysts.

Our work deals with synthesis of MOFs containing cerium cations, of UiO-66 and MOF-808 topology, that could be used as catalyst in reactions allowing CO_2 conversion. According to very good redox properties of cerium, its introduction to MOF structure is a chance to improve both the adsorptive and catalytic properties of parent material. Moreover, Ce-based MOFs containing Ce on +3 and +4 oxidation state can be considered bifunctional because Ce4+ cations act as Lewis acid sites, while Ce3+ act as Lewis basic sites responsible for adsorption of CO_2.

In presented work we would like to demonstrate the influence of synthesis method on the physico-chemical properties of Ce containing MOFs and their ability to adsorb (reversibly and irreversibly) CO_2. The impact of synthesis parameters on crystallographic structure (XRD), composition (XPS, IR), textural properties (N2 sorption), morphology (SEM), thermal stability (TGA), and CO_2 sorption capacity of these materials will be presented. Moreover, the results of catalytic tests of CO_2 hydrogenation to methanol over selected MOFs will be shown.

Audience Take Away:

- The insight into new, Ce containing MOF materials as potential, new catalysts for CO_2 conversion.
- Cognition of the dependence of synthesis method/synthesis parameters on the properties of Ce containing MOFs.
- Presented results may be used by the audience whilst planning synthesis of Ce containing MOFs for obtaining materials of a precise crystallographic structure, textural properties, chemical composition (especially crucial in terms of the Ce^{3+}/Ce^{4+} content and further catalytic performance).

Biography

Michalina Stawowy is a PhD student in the Department of Fuel Chemistry and Technology at the Wrocław University of Science and Technology. Her field of interest are new cerium containing mono-, bi- and polymetallic MOFs for carbon dioxide adsorption and its catalytic conversion e.g. to methanol.

Modelling hyaluronan degradation by *Streptococcus pneumoniae* hyaluronate lyase

Vinh Q. Mai[1, 2*], **Tuoi T. Vo**[3], **Martin Meere**[1]
[1]Department of Applied Mathematics, NUI Galway, Ireland
[2]Department of Mathematics, Thu Dau Mot University, Binhduong, Vietnam
[3]MACSI, Department of Mathematics and Statistics, University of Limerick, Limerick, Ireland.

Hyaluronic acid (Hyaluronan) is a linear, high molecular weight polysaccharide that forms an important component of the extracellular matrix. It is an excellent biomaterial, and it is increasingly being used in biotechnology, biomedical applications, and drug delivery. Polymer chains of hyaluronan occur in many different lengths in nature, and can be as large as multiples of ten thousand. Since the biological function of a hyaluronan chain often depends on its molecular weight, it is of value for applications to develop reliable quantitative descriptions of the degradation processes of hyaluronan. In particular, the development of such models should assist with the rational design of production processes to create polymer chains in a given molecular weight category for a specific application. In this paper, we propose a new mathematical model for the degradation of hyaluronan by the enzyme streptococcus pneumoniae hyaluronate lyase. The model is based on a processive kinetic mechanism and consists of a coupled system of nonlinear ordinary differential equations for the species of interest. The model parameters are estimated using published experimental data, and good agreement between theory and experiment is found. Numerical experimentation and a Sobol global sensitivity analysis reveal that the key model parameters are the initial enzyme concentration and the rate constants for enzyme adsorption and catalysis.

Audience Take Away:

- Have an appreciation of why hyaluronan is an important and interesting biopolymer.
- Understand that the biological function of a hyaluronan chain can depend on its length.
- Have seen how to construct a mathematical model for the degradation of hyaluronan by a bacterial enzyme, and appreciate why a mathematical model can assist with the rational design of production processes to create polymer fragments of a given length.
- Have seen how a sensitivity analysis can be used to identify the dominant mechanisms in the degradation process.

Biography

Vinh Q. Mai is an applied mathematics PhD student at NUI, Galway, where he was awarded a scholarship by the College of Science. He has been a lecturer in mathematics at the Thu Dau Mot University since he left a lecturing position at the Angiang University in 2010. He earned a Masters degree in Geometry and Topology at the Hanoi National University of Education in 2008.

Adsorption of perfluorinated surfactants on activated carbon: Role of the adsorbent's surface chemistry

Navid Saeidi*, Ph.D. Student, Anett Georgi, Frank-Dieter Kopinke
Department of Environmental Engineering, Helmholtz Center for Environmental Research-UFZ, Leipzig, Germany

Perfluorinated alkyl surfactants (PFAS) are a class of anthropogenic organofluorine compounds in which each hydrogen atom on the alkyl chain is replaced by a fluorine atom. All PFAS contain a hydrophilic head group and a hydrophobic perfluorinated tail. So they have unique distinct amphiphilic properties compared to conventional hydrocarbon-based surfactants, enabling their use in various application areas. In addition, the mentioned properties make them persistent, bioaccumulative and almost ubiquitously distributed in aquatic environments. Their widespread occurrence in the environment may produce long-term and extensive harm to human and wildlife, which has been confirmed in recent years. Therefore, efficient removal of PFAS from water is of vital importance. Adsorption particularly by utilization of activated carbon (AC) is recognized as a promising technique for this purpose. However, it has been reported that variation in adsorption performance of various AC products is much more pronounced for PFAS than known for conventional non-polar contaminants. An appropriate selection of activated carbon for an efficient removal of PFAS has not been discussed in detail yet.

In this presentation, the key chemical characteristics of AC which are crucial for optimal adsorption of PFAS will be discussed. Actually, several activated carbon felts (ACFs) were characterized with various techniques including nitrogen adsorption-desorption analysis for determination of porosity, light microscopy to measure the fiber's diameter, determination of point of zero net proton charge (PZC) and total acidity by Boehm titration method, temperature-programmed desorption (TPD) for quantification of O-containing functional groups, as well as anion and cation exchange capacity of the ACFs by the respective standard methods. Among these ACFs, four of them having different surface chemistries but the same porosity and fiber's diameter were selected and applied for next experiments. A series of adsorption experiments were performed to study the role of surface chemistry of AC on equilibria and kinetics of PFAS adsorption and to describe them by appropriate models. In addition, adsorption of PFAS on the ACFs in presence of natural organic matter (NOM) and different concentrations of metal cations (monovalent and divalent) were investigated. The results proved that there was a significant difference between adsorption affinities of PFAS on these four ACFs even in presence of NOM and different concentrations of metal cations. The most influencing chemical characteristics of the ACFs in adsorption of PFAS were identified. After that, it was tried to take advantage of the results obtained here to chemically modify the ACF with lowest affinity in adsorption of PFAS. The modified ACF sample showed a strongly enhanced adsorption whereby Freundlich isotherm coefficients of the two PFAS under study (perfluorooctanoic acid and perfluorobutanoic acid) increased by almost 3 and 2 orders of magnitude, respectively, compared to the original ACF.

Audience Take Away:

- The audience will learn how to characterize chemically the activated carbon and extend these methods to other carbon-based porous materials.
- They will learn how to find and address the key characteristics of adsorbents for an efficient removal of target pollutants from water, in particular perfluorinated surfactants.
- The audience from industry will realize which kind of activated carbon is the best for adsorption of perfluorinated surfactants for practical applications.
- The researchers will gain mechanistic understanding of possible solute-adsorbent interactions especially for amphiphilic solutes.

Biography

The presenter is from Iran. He studied chemical engineering in Semnan university of Iran. After finishing his master, he won a DAAD scholarship for conducting a PhD study in Germany. Then, he started his PhD in 2016 in the Department of Environmental Engineering of Helmholtz Center for Environmental Research-UFZ under supervision of Prof. Frank-Dieter Kopinke and Dr. Anett Georgi. He is doing research on efficient removal of emerging micropollutants from water and interactions between organic pollutants and carbon-based adsorbents.

Fisher-Tropsh synthesis in the presence of dispersed catalysts on the basis of ir-pyrolysed metal-polymer systems

Ivantsov Mikhail Ivanovich[1]*, Khadziev S.N[2], Kulikova M.V[3], Ph.D.
[1]Junior researcher, A.V.Topchiev Institute of Petrochemical Synthesis, RAS (TIPS RAS), Russian Federation
[2]D.Sc. in Chemistry, Professor, Academician of RAS, A.V.Topchiev Institute of Petrochemical Synthesis, RAS (TIPS RAS), Russian Federation
[3]Head scientist researcher, Chief of the Department, A.V.Topchiev Institute of Petrochemical Synthesis, RAS (TIPS RAS), Russian Federation

The synthesis of synthetic liquid hydrocarbons from synthesis gas by Fischer-Tropsch synthesis (SFT) is central part of most XTL (GTL, CTL, BTL) processes. Constant instability in the oil market and relentless reduction of reserves of light extracted oil make research of the processes of converting any carbon-containing raw material into hydrocarbons relevant. One of the trends in the development of SFT technologies is search of new catalytic systems, and also development of nanotechnologies promoting emergence of new unique materials - nanocomposites, one of features of which is synergy of the matrix and the dispersed component.

For the first time, a number of nanoscale cobalt- and iron-polymer catalytic systems based on cellulose, polyvinyl alcohol, and polystyrene were synthesized for Fischer-Tropsch synthesis. Their catalytic activity in the synthesis of liquid hydrocarbons from CO and H_2 was established.

It is found that the composite materials produced by pyrolysis of metal salt compounds and polymers mixes can be formed by polycondensation or destructive scheme. It is established that composite materials represent evenly distributed metal-containing nanoparticles in pyrolyzed matrix, and the phase structure and size of particles depends on temperature of thermolysis.

It is shown that during synthesis of the composite material, nanoparticles which show activity in the Fischer-Tropsch synthesis without the preliminary reduction step distributed in the pyrolyzed matrix are formed. At the same time, the CO conversion on samples containing cellulose, PAN, PVA in it composition, aspired to 100%.

It is revealed that nature of the initial polymer component of composite material has a significant effect on the catalytic properties of composites, with systems forming a system of polyconjugate bonds having the greatest activity, which can cause high contact productivity (up to 4800 g / kgMe.h).

It is assumed that the matrix formed during the synthesis of the composite is not only a dispersed medium for nanoparticles, but also a component of the catalytic center at which dissociative adsorption takes place and subsequent hydrogenation of carbon monoxide. This work was done as part of TIPS RAS State Plan.

Audience Take Away:

- The audience will learns about new types of dispersed catalysts that have high activity in SFT
- The audience working in the region will be able to apply new approaches to the synthesis of catalytic systems
- The audience will learn about the application of modern physical and chemical methods for studying of solid dispersed systems

Biography

Mikhail Ivantsov: 1990 year of birth; 2012 year – graduated from chemistry department of Lomonosov MSU with qualification of Specialist in Chemistry; in 2012 - 2016 student of graduate school of Lomonosov MSU chemistry department in kinetics and catalysis. 2013 to the present – junior Researcher of A.V.Topchiev Institute of Petrochemical Synthesis, RAS (TIPS RAS).

Tuning acidity in metal organic frameworks-based catalysts for enhanced production of Butyl Butyrate as a biofuel additive

Asmaa Jrad[1]*, Ph.D. student, Belal. J. Abu Tarboush[1], Ph.D., Mohamad Hmadeh[2], Ph.D., Mohammad Ahmad[1], Ph.D.
[1]Department of Chemical and Petroleum Engineering, Faculty of Engineering and Architecture, American University of Beirut P.O.Box, 11-0236, Beirut, Lebanon
[2]Department of Chemistry, Faculty of Arts and Sciences, American University of Beirut P.O.Box, 11-0236, Beirut, Lebanon

In an attempt to optimize the production of biofuel additives from biomass-derived components, different structures of metal organic frameworks (MOFs) were synthesized to serve as catalysts for the esterification reaction of butyric acid with butanol to produce a green fuel additive, butyl butyrate. The thrust of this study is to understand at a fundamental level the relations between the structure, properties and catalytic performance of champion materials that confer upon them the capacity to function as efficient esterification catalysts. For this purpose, a variety of MOFs were synthesized and fully characterized by X-ray diffraction, electron microscopy, Brunauer–Emmett–Teller (BET) measurements and thermogravimetric analysis. Their acid density was evaluated using back titrations. All prepared MOFs were efficiently used as catalysts of the liquid-phase esterification reaction for the production of butyl butyrate. Interestingly, 91% conversion was achieved by employing one of the most acidic members as a heterogeneous catalyst, which is very close to the 96% conversion obtained by the conventional homogeneous liquid catalyst H_2SO_4. This exceptional rate was attributed to its superior acid density which was found to be the key factor to high conversion. All MOFs were easily separated from the reaction medium, recycled, and reused without significant loss in activity after at least four cycles. XRD analysis and acidity test of the recycled MOFs confirmed that their acidity and crystallinity were retained. With this knowledge, catalytic conversion rates and efficiencies of MOFs can be engineered from a laboratory prototype and optimized by tuning the functional groups of the organic linkers to serve as effective catalysts for the production of fine chemicals such as biofuels.

Audience Take Away:

- Given that the work presented focuses on the design of metal-organic frameworks to serve a specific catalytic reaction, the foundings discussed will inspire and encourage researchers working in catalysis to optimize the structure of metal organic frameworks for their specific and relevant catalytic application in any chemical reaction.
- The work presented will highlight the means by which MOFs' properties and active sites could be modified for a specific application. This would pave the road for other researchers wishing to develop MOFs-based catalysts.
- The research shows a new class of heterogeneous and recyclable catalysts that could be of interest to researchers working for the industrial sector.

Biography

Asmaa Jrad is a PhD student working on catalysis and chemical reaction engineering at the American University of Beirut, Faculty of Engineering and Architecture, Chemical and Petroleum Engineering Department. She graduated with honors from the Lebanese University with a BE degree in chemical and petrochemical engineering, and got her Masters degree in engineering from the American University of Beirut. Currently she is leading a research group working on developping catalysts from metal-organic frameworks to produce higher chemicals for the energy and biofuel sector from bio-mass derived feedstock.

Catalysis of Zeolitic Imidazole framework-7: Non-Phosgene route for Methyl N-Phenyl Carbamate synthesis

Deliana Dahnum[1,2]*, Hyunjoo Lee[1,2], Ph.D.
[1]Clean Energy Center, Korea Institute of Science and Technology, Seoul 02792, Republic of Korea
[2]Division of Energy & Environment Technology, KIST School, Korea University of Science and Technology, Seoul 02792, Republic of Korea

Isocyanates are widely used in industries as important precursors for the synthesis of polyurethane, pesticides, and herbicides. These materials are commercially produced by the reaction between amine and phosgene which is known as un-environmental friendly due to their drawbacks, including toxicity, corrosion problem, and yielding salt and organic halogen compound as a waste. Hence, considering environmental pollution and safety issues, many of studies are accomplished to develop a non-phosgene reaction as one of an alternative route. Synthesis Methyl N-phenyl carbamate (MPC) as an intermediate precursor of isocyanate is one of the attractive process, which is conducted by reacting aniline and dimethyl carbonate (DMC). DMC itself is known as an environmentally benign building block and serves as a methoxycarbonylation agent. In this study, Zeolitic Imidazole Framework-7 (ZIF-7) has been used as a catalyst for methoxycarbonylation reaction of aniline and DMC to produce MPC. ZIF-7 was prepared by the solvothermal method, in which four types of difference zinc precursor, including $Zn(OAc)_2$, $ZnCl_2$, $Zn(NO_3)_2$, and $ZnBr_2$ reacts with benzimidazole. The results show that ZIF-7 synthesized by zinc acetate precursor exhibits the highest activity among other precursors. The aniline conversion and MPC yield achieve 97.53% and 84.42%, respectively, while the reaction is conducted at 190°C for 2 hours. Reusability study confirmed that catalytic activity of catalyst could be maintained during 4 times reuses. The catalyst was characterized by Fourier Transform Infrared (FT-IR), Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD), CHON elemental analysis, Inductively Coupled Plasma Atomic Emission Spectroscopy (ICP-EAS), and proton NMR.

Audience Take Away:

- This study could be used as an alternative process producing isocyanate precursor which is more friendly for environment
- A new application has been developed for Zeolitic Imidazole Framework as a catalyst for methoxycarbonylation reaction, so might be other application can be initiated in the future research.

Biography

Deliana Dahnum received B.S degree in chemical engineering from Sepuluh Nopember Institute of Technology, Indonesia. Currently, she is a Ph.D candidate in integrative course majored energy & environmental technology in KIST School, Republic of Korea. Her research works are related to catalyst synthesis and biomass conversion.

CONTENTS

Electrochemical optimization of platinum and gold nanogap interdigitated electrode arrays

Volha Matylitskaya*[1], Ph.D., Lenka Gajdosova[1], Ph.D., Elisabeth Kostal[1], Can Dincer[2], Stefan Partel[1]
[1]Research center for microtechnology, Vorarlberg University of Applied Sciences, 6850 Dornbirn, Austria
[2]Dr.-Ing., Department of Microsystem Engineering (IMTEK), University of Freiburg, Freiburg 79110, Germany; Department of Bioengineering, Royal School of Mines, Imperial College London, London SW7 2AZ, Great Britain

In this work we compare the electrochemical behavior of the fabricated platinum and gold nanogap interdigitated electrode arrays (nIDAs) for Lab-on-a-Chip (LoC) applications. Chronoamperometric measurements were carried out to achieve a signal amplification compared to a single electrode configuration. In chronoamperometric measurements a significant amplification can be achieved by interdigitated electrode arrays in combination with a reversible redox process. The attainable signal amplification depends on the electrode distance, the smaller the electrode gap the higher the amplification. Therefore, a gap size in the nanometer range is desired for the fabricated electrode array. Conventional microfabrication techniques were used for the fabrication of the sensor chip with adjustable nanogaps.

Two redox couples, ferrocenemethanol (FcMeOH) and p-aminophenol (pAP), were selected for the electrochemical experiments. The redox potentials of both tested substances were determined by cyclic voltammetry. The scan ranges from 0.0 V to +0.3 V for FcMeOH and from -0.3 to +0.4 V for pAP (vs. Ag/AgCl as reference electrode) were determined as optimum. Suitable cleaning procedures were developed and optimized to suit the different requirements for Pt and Au chips. Cleaning of Pt nIDAs (regardless of the redox couples to be used) includes an initial treatment in O_2 plasma and an electrochemical cleaning. For the Au chips, O_2 plasma cleaning alone is sufficient. No influence of the electrochemical cleaning in 0.1 M PBS (phosphate buffered saline) on the signal amplification achievable by the Au chips was observed. With the presented process a maximum amplification of 160 for Pt and 130 for Au can be achieved. This is the highest published amplification in bulk solution for the measurements with IDAs.

The results show that not only high signal amplification but also high current efficiency above 99 % has been reached for both Au and Pt nIDAS with both tested solutions FcMeOH and pAP. High signal amplification and current efficiency make the fabricated nIDA an exellent candidate for further ELISA experiments.

Audience Take Away:

- The fabricated nIDAs are suitable for use as electrochemical biosensor. Electrochemical biosensors provide an attractive way to analyze the content of a biological sample due to the direct conversion of a biological event to an electrical signal. Therefore development and electrochemical characterization of such kind of screening tools are very important for different scientific areas.
- The gap size of the tested IDAs is in nanometer range. Normally when the gap and electrode size shrinks down to submicron and nanometer sizes, more advanced and expensive manufacturing technologies are required. The characterized IDAs with adjustable nanogaps between the finger electrodes were created using conventional and at the same time low cost microfabrication techniques.
- Normally the most critical step by the fabrication of nIDAs is the lift-off step. With the used fabrication sequence, it is possible to generate gaps in the nanometer range without any lift-off process.
- We have also shown which parameters are significant for the achievable amplification at the chronoamperometric measurements with platinum and gold nIDAs.
- Formation of the polymer layer during redox cycling with p-aminophenol was observed. An influence of the formed polymer film on achievable amplification was investigated.

Biography

Volha Matylitskaya, studied chemistry at P.M. Mascherov University in Vitebsk (Belarus). She received her PhD degree from J.W. Goethe University of Frankfurt/Main (Germany) in 2009. The subject of her dissertation was the study the possibility of niobium oxynitride formation by Rapid Thermal Processing. During her PhD Dr. Matylitskaya dealt with the solid state chemistry as well as with the methods of the solid state analysis. Ms. Matylitskaya currently works at the Research Center for Microtechnology at the University of Applied Sciences Vorarlberg (Austria). The current focus of her research is the electrochemical characterization of the fabricated interdigital electrode arrays and investigation of their potential for lab-on-a-chip applications.

CONTENTS

Tio$_2$ - Carbon derivatives composite photocatalyst for advanced and affordable wastewater treatment

Anca Duta*, Cristina Bogatu, Maria Covei, Ioana Tismanar
R&D Centre, Renewable Energy and Recycling, Transilvania University of Brasov, Romania

The quest for novel efficient and affordable wastewater treatment processes brought photocatalysis into the focus. Highly efficient photocatalysis is based on wide band gap semiconductors that can depollute the wastewater even at low pollutant concentrations (at the ppm range) but above the discharge limit. Among the photocatalysts TiO_2 is considered as one of the best candidates in the photocatalytic removal of pollutants during the advanced wastewater treatment, due to its stability in the aqueous media and its lack of toxicity. However, the wide band gap of TiO_2 makes its activation possible only when using UV radiation. This is why, the challenge to develop up-scalable and affordable processes lead to the development of various solutions, based on composite layers that make the TiO_2 component VIS-active; one of the recent attempts is to develop TiO_2-graphene composite structures that support a better charge separation and reduce the electron-hole recombination in TiO_2, thus better supporting the photocatalytic reaction mechanism. These composites are mostly reported to be obtained using sol-gel or hydrothermal synthesis, but this paper will report on thin composite layers of TiO_2 and reduced graphene oxide (rGO) obtained by Spray Pyrolysis Deposition. The thin films are further tested in the methylene blue removal (according to the standard ISO 10678; 2010) and the results show that the process runs with promising efficiency when irradiated with solar radiation (irradiance higher then 600 W/m2). The influence of the synthesis conditions is investigated and the results show the optimum rGO content in the composite is of 1%. As the composite photocatalyst needs only solar radiation, the process is affordable and the results can be used also in developing self-cleaning coatings with similar composition.

Audience Take Away:

- Novel synthesis and deposition method(s) for composite thin films with TiO_2 matrix.
- The key requirements that govern the synthesis of these type of thin films.
- The photocatalytic performance of these thin films with applications in advanced wastewater treatment and possible in self-cleaning surfaces.

The presentation will outline the experimental conditions that supported the results and the way how the compatibility challenges among the composite components were solved.

Biography

Anca Duta (b. 1961) is Professor in the Transilvania University of Brasov, Romania and Ph.D. supervisor in Materials Science. Her activity focuses on solar energy materials used in solid state solar cells, solar-thermal coatings and in photocatalysis and is part of the H2020 group of experts on this topic(s). Her recent work on VIS-active photocatalytic materials focuses on the development of thin films, stable in water, with a structure similar to solid state solar cells that are efficient in organic pollutants removal from wastewater (e.g. TiO2/CZTS or TiO2/CIS). Further on, the development of VIS-active composite thin films included also graphene and graphene derivatives deposited on TiO2 to get VIS-active materials for advanced wastewater treatment or for self-cleaning coatings.

Molybdenum disulfide (MoS_2) based photocatalysts for photocatalytic hydrogen production

S. V. Prabhakar Vattikuti*, Ph.D., Jaesool Shim, Ph.D.
School of Mechanical Engineering, Yeungnam University, Gyeongsan, South Korea, 712-749

Modern advancement in design of the efficient visible driven photocatalyst for solar-to-hydrogen generation has been expanded much consideration due to fossil fuels crisis, which convert and store solar energy into chemical fuels. In view point of economic and large-scale application, semiconductor photocatalyst with high stability and efficiency should be required. However, a numerous number of materials have been discovered, challenges still remain for the commercialization. Among the enormous number of materials, layered structured transition metal dichalcogenides (TMDs) based photocatalyst have been shown attractive performance in photocatalytic process owing to their suitable narrow bandgaps, high absorption capacity and fast carrier transport properties. This review to be covered the physicochemical features and recent advancements of various layered structured TMDs based photocatalysts, especially MoS2 and various approaches to improve the photocatalytic reaction and stability by coupling active carbon materials including graphene, carbon nanotubes (CNTs), active carbon, precious metals and other metal oxides, etc. We rely on this review can reveal some insights of fundamental concepts of role of active chemical species during the solar-to hydrogen conversion processes and their influences in enhanced performance on PEC water splitting.

Audience Take Away:

- To understand the important of 2D materials in catalysis
- To understand the latest advancements in development of photocatalysts for water splitting
- To educate the possible mechanism involved in photocatalytic reactions
- To understand the modern techniques to enhance the photocatalytic efficiency and stability of MoS2 photocatalyst

Biography

Vattikuti has completed his PhD degree in Nanomaterials and Coatings from Chung Hua University, Taiwan in the year 2010. He received one year postdoctoral fellowship from Yeungnam University (2014-2015). Currently he is International assistant professor in School of mechanical Engineering, Yeungnam University, South Korea. He has published more than 60 papers in reputed journals and has been serving as a reviewer of repute journals. He received three years fund from National Research foundation of Korea (NRF-Korea) (2017-2020). His research focuses on transition metal Chalcogenide materials for energy and photocatalytic applications.

Polymeric metal Schiff base complexes as catalysts for photoelectrocatalytic hydrogen peroxide production

Oleg Levin*, Ph.D., M. P. Karushev, Ph.D., E. A. Alekseeva, Ph.D., A. S. Konev, Ph.D.
St. Petersburg State University, Russian Federation

Hydrogen peroxide represents clean and convenient energy source for fuel cells. H_2O_2 is mostly produced in industry by anthraquinone process, where 2-alkylanthraquinone is reduced by Pd-catalyzed hydrogenation to 2-alkylanthrahydroquinone, which undergoes autoxidation in the presence of oxygen giving eventually hydrogen peroxide and resuming 2-alkylanthraquinone. Photocatalytic production of hydrogen peroxide by photo induced reduction of molecular oxygen represents an appealing alternative to anthraquinone process, as it might decrease the energy consumption and reduce the production cost. In this work, we report our study on possible application of metal Schiff base complexes as cheap photoredox catalysts for H_2O_2 production. Activity of $[M^{II}(L)]n$ complexes, where M is Ni, Cu or Pd and L is a tetradentate N,N,O,O ligand of Schiff base family, in the photoelectrocatalytic reduction of molecular oxygen to hydrogen peroxide has been demonstrated. The effect of pH of the medium and the ligand in the coordination sphere on the reaction rate and the photocurrent produced were studied, the maximal photocurrent and H_2O_2 concentrations achieved comprising 23 μA/cm2 and 1.2 mM respectively. The efficiency of H_2O_2 production reaches 97% after 6 hours of operation. Taking into account that complex is obtained from cheap commercial chemicals by using simple experimental techniques, the observed performance makes this material perspective for practical applications.

Audience Take Away:

- Artificial photosynthesis of hydrogen peroxide is one of convinient ways to convert solar energy into chemical or electrical energy.
- The research describes a new class of photoactive materials for combined electrical energy production and hydrogen peroxide artificial photosynthesis.
- Presented materials may be used for further development of photoelectrochemical systems.

Biography

Dr. Sci. Oleg V. Levin, Associate Professor of electrochemistry, Institute of chemistry, St. Petersburg State University is a specialist in the field of electrochemistry of electroactive polymers. Studies carried out by O. Levin, contribute to the development of new organic and hybrid materials for electrochemical power sources. Principal scientific achievements of O.V. Levin are: development of charge transfer model in electroactive polymer films; creating new formulations of binders for Li-ion batteries; development of new organic active materials for batteries, supercapacitors and photovoltaic cells.

Particulate photocatalyst sheets for scalable Z-scheme photocatalytic water splitting

Siang-Piao Chai*, Ph.D., Boon-Junn Ng, Lutfi Kurnianditia Putri, Pooria Pasbakhsh, Ph.D.
Monash University, Malaysia

Owing to the energy and environmental issues become more apparent on a worldwide scale, a transition of energy supply from conventional fossil fuels to a more promising carrier, namely hydrogen (H_2), is anticipated in the near future. Photocatalytic water splitting is one of the many endeavors in harvesting H_2 fuel using the abundant energy from the Sun. Cutting edge research within the field focuses on the biomimetic artificial Z-scheme photocatalysis which comprises of the ingenious arrangement of a HEP (PS I) and an OEP (PS II) connected by an electron mediator. As of recent, scalable photocatalytic water splitting has been witnessed in particulate photocatalyst sheets inspired by Z-schematic HEP-conductive layer-OEP system. One of the major challenges in developing an efficient Z-scheme photocatalyst sheets is establishing efficient interparticle electron transfer between HEP and OEP, which are embedded on the conductive layer. A proof-of-principle demonstration on Z-scheme particulate photocatalyst sheets system speculates that the HEP-OEP layers often thickly stacked on the conductive layer, which greatly suppress the electron relaying within the system. In this study, the implication of nitrogen-doped carbon nanotubes (N-CNTs) was investigated as conductive mediator layer to bridge twinned $Zn_{0.5}Cd_{0.5}S$ (HEP) and Bi_4NbO_8Cl (OEP) in Z-scheme photocatalytic water splitting. Annealing of the HEP-OEP layers on N-CNTs sheet and surface modification was done to improve electron transfer within the particulate sheets. The optimized particulate photocatalyst sheets exhibited outstanding overall water splitting to yield 10.8 mol h-1 of H_2 and 5.2 mol h^{-1} of O_2 under simulated solar light irradiation. In all, these findings could extend the electron mediator candidates to a larger horizon and pave way in future solar energy augmentation.

Audience Take Away:

- A method to convert solar energy to chemical energy through water splitting
- Strategies to develop efficient Z-scheme photocatalysts
- Know how on the photocatalytic process and mechanism to split water effectively into hydrogen and oxygen

Biography

Chai Siang Piao is currently a Professor and the Deputy Head of School (Research) for School of Engineering as well as the Head of Nano-Analytical Platform at Monash University Malaysia. Prof. Chai is an active researcher in the areas of catalysis, photocatalysis, reaction engineering, and advanced functional materials. His current research interests are centered on the development of advanced hybrid nanomaterials for environmental remediation and renewable fuels in photocatalysis. He has published more than 130 ISI-papers, accumulated total citations of more than 5000 and H-index over 34.

CONTENTS

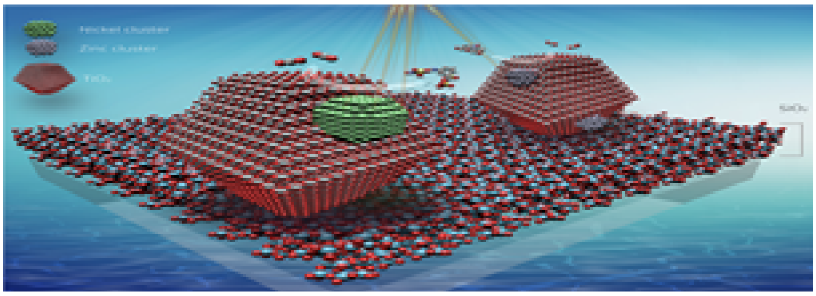
Effects of surface Ni and Zn oxo-nanoclusters on Tio$_2$ for solar light photocatalysis

Andraž Šuligoj, Ph.D.[1]*., Nataša Novak Tušar[2], Ph.D., Iztok Arčon[3], Urška Lavrenčič Štangar[4], Ph.D.
[1]National Institute of Chemistry, Slovenia and Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia
[2]National Institute of Chemistry, Slovenia
[3]University of Nova Gorica, Slovenia
[4]Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia

Titanium dioxide has been widely used as an antimicrobial agent, UV-filter and catalyst for pollution abatement. Herein, surface modifications with selected transition metals (Me) over colloidal TiO_2 nanoparticles and immobilization with a colloidal SiO_2 binder as composite films ($MeTiO_2/SiO_2$)on a glass carrier were used to enhance solar-light photoactivity. Colloidal TiO_2 nanoparticles were modified by loading selected transition metals (Me: Mn, Fe, Co, Ni, Cu, and Zn) in the form of chlorides on their surface. They were present primarily as oxo-nanoclusters and a portion as metal oxides.

The structural characteristics of bare TiO_2 were preserved up to an optimal metal loading of 0.5wt%. We have shown in situ that metal-oxo-nanoclusters with a redox potential close to that of $O_2/O_2^{\bullet-}$ were able to function as co-catalysts on the TiO_2 surface which were excited by solar-light irradiation. The materials were tested for photocatalytic activity by two opposite methods; one detecting $O_2^{\bullet-}$ (reduction, Rz ink test) while the other detecting •OH (oxidation, terephthalic acid test). It was shown that the enhancement of the solar-light activity of TiO_2 by the deposition of transition metal oxo-nanoclusters on the surface depends strongly on the combination of the reduction potential of such species and appropriate band positions of their oxides. The latter prevented excessive self-recombination of the photogenerated charge carriers by the nanoclusters in Ni and Zn modification, which was probably the case in other metal modifications.

Overall, only Ni modification had a positive effect on solar photoactivity in both oxidation and reduction reactions.



Audience Take Away:

- The aspects of surface modification of TiO_2 will be covered, with fundamental reasons for enhanced solar light activity explained,
- The general rules for further successful modifications will be given and lastly,
- Some insights into successful applications of such materials in form of thick films will be given.

Biography

Andraž Šuligoj is working in the field of applied photocatalysis. He started with the development of highly UV-active films on metal substrates (Fe, Al) for which he developed a silica protective layer, which was later patented. He then switched to designing novel systems combining TiO_2 anatase and mesoporous silica for air cleaning applications. Lately, he is focused on designing solar light-active TiO_2 by employing green and facile incipient wet impregnation, resulting in the surface modification of TiO_2, giving rise to novel hetero-junctions. Thus he is studying the structure-activity relationship, with the focus on nano-clusters deposited on the anatase surface.

CONTENTS

Molecular catalysts for water oxidation in a homogenous solution and heterogeneous surface

Masayuki Yagi
Niigata University, Japan

Water splitting by sunlight into molecular hydrogen and oxygen in artificial photosynthesis is a promising technology to settle the energy and environmental issues. In this context, much effort has been paid for development of molecular catalysts for water oxidation inspired by the oxygen-evolving complex in photosystem II. Herein we report unique synthesis of a new series of dinuclear ruthenium (II) complexes using photoisomerization of a mononuclear complex. The activity and mechanism of electrocatalytic water oxidation by these derivatives in homogeneous solution and heterogeneous surface will be discussed.

Biography

Masayuki Yagi received his Ph.D. from Saitama University. He joined the faculty of Niigata University (Japan) in 1996 and was promoted to Associate Professor of Chemistry in the following year. He has been Professor of Materials Science and Technology since 2009. From 1999 to 2001, he worked as a Visiting Fellow at Princeton University with support from the JSPS program. From 2009 to 2013, he worked as a PRESTO fellow at JST.

In-situ Raman spectroscopic monitoring of mechanochemical preparations of energy-related materials

Nikola Biliškov*, Ph.D., Igor Milanović, Ph.D., Ivan Halasz, Ph.D.
Ruđer Bošković Institute, Zagreb, Croatia

Mechanochemical reactions by ball milling are becoming increasingly popular across a wide range of chemical sciences, but understanding and evaluation of the processes included in these processes remain a persistent challenge. It is important to note that ex-situ measurements can give a distorted picture on the investigated system, since temporary stopping of the reaction and opening of the milling jar can significantly change the reaction pathway. Thus, it was important to develop the techniques able to give an insight into the mechanochemical reactions in-situ and in real time. Obviously, the understanding of mechanochemical processes, especially the detailed understanding of mechanistic details, is crucial for optimization of these reactions. Recently, a few techniques that allow in-situ monitoring of ball milling reaction in real time are developed and well established. For now, they include in-situ XRD and Raman spectroscopic monitoring, as well as follow-up of the temperature inside the milling jar during reaction. Here we concentrate only on Raman spectroscopic monitoring, since exclusively this technique was applied to synthesis energy-related materials.

For the first time, we applied one of these techniques, Raman spectroscopy, in order to follow up the mechanochemical synthesis of materials for solid-state hydrogen storage. More specifically, the technique was applied to a series single- and bimetallic amidoboranes of MAB, MAB•AB, M_2MgAB4 and M_2CaAB_4 (M = Li, Na ; AB = NH_3BH_3) composition, that were prepared and thoroughly characterized. A detailed analysis of spectral data revealed that a common two-step mechanism takes place through MAB•AB adducts as a key intermediate phase.

In addition, the technique was applied to mechanochemical preparation and exfoliation of the systems based on 2D transition metal dichalcogenides of the TX_2 composition (T = Mo, W; X = S, Se, Te), as well as exfoliation of TO_3 type transition metal oxides and graphene by use of widely accessible exfoliants, such as oxalic acid, sugars, ammonia borane etc.

Our results show that Raman spectroscopic monitoring of ball milling reactions undoubtedly provides a unique insight into the mechanochemical reactions under run, in real time.

Audience Take Away:

- Presentation of a relatively novel technique for in-situ monitoring of mechanochemical reactions
- Using the mechanochemical preparation of energy-related systems as an example, the application and strengths of this technique will be presented
- A few novel chemical systems for hydrogen storage will be presented.
- The applicability and advances of the monitoring techniques will be presented.
- These techniques are generally applicable to a wide range of ball milling reactions, with a high opportunity for further advances by addition of measurement of other parameters relevant for chemical reactivity.

Biography

Born September 17, 1974 in Pula, Croatia. In 1999 Masters degree of inorganic chemistry at Faculty of Sciences, University of Zagreb; thesis at Faculty of Science in Zagreb. 2009 PhD degree in physical chemistry at Ruđer Bošković Institute, Zagreb. 2012 Research associate at the Laboratory of Solid State and Complex Compounds Chemistry, Division of Materials Chemistry, Ruđer Bošković Institute, Zagreb 2014 Visiting scientist at EMPA, Dept. Hydrogen and Energy, Dübendorf, Switzerland and at Hungarian Academy of Sciences.

Ozonation in a multi-orifice oscillatory baffled column

Marco Paulo Gomes Sousa Lucas[1]*, M.Sc, Ph.D., Nuno Reis[2], Ph.D., Gianluca Li Puma[3], MPhil, Ph.D.
[1]Universidade de Trás-os-Montes e Alto Douro, Portugal
[2]University of Bath, UK
[3]Loughborough University, UK

A novel approach for the intensification of ozonation of water and wastewater is presented using a highly efficient and compact Multi-Orifice Oscillatory Baffled Column (MOBC) ozonation contactor. The MOBC uniquely yielded full (i.e. 100%) use of the ozone supplied with a very short (2.25 min) liquid contact time under continuous operation and without the need of further gas-liquid contacting equipment downstream from the MOBC. The increased performance of the MOBC ozonation reactor was benchmarked against a bubble column (BC) design and resulted in 20% increase on the rate of p-hydroxybenzoic acid (p-HBA) degradation, 75% increase in the rate of mineralization of p-HBA per mole of ozone consumed, and 3.2-fold increase in the rate of mineralization of p-HBA per mole of ozone supplied. This results from the very small size of bubbles (few hundreds of microns) and enhanced gas-liquid mass transfer and hold-up generated in the presence of small fluid pulsations and orifice baffles. Experiments with two pharmaceutical compounds (Diclofenac and Caffeine) were also performed.

- Water ozonation intensification in a Multi-Orifice Oscillatory Baffled Column;
- Higher rates of ozone utilization in a highly compact device;
- MOBC ozonation reactor is benchmarked against a bubble column;
- MOBC allows a reduction of 5-fold to one-order of magnitude in reactor volume.

Biography

Marco S. Lucas is principal investigator at University of Trás-os-Montes and Alto Douro. Holds a PhD in Chemistry, a Master in Environmental Technology and a degree in Environmental Engineering. Its main research interests are i) water and wastewater treatment, ii) advanced oxidation processes, iii) environmental chemistry, iv) adsorption and v) biologic processes. Until now he has published 33 papers in top-ranked and peer-reviewed journals, 1 patent, 1 book chapter and more than 100 conference proceedings and communications. Has an h-index of 15 and more than 1350 citations. Has been awarded with a Marie Curie Experienced Researcher (IF) by the European Commission (Loughborough University, UK) and three research prizes.

Novel Ir(III)-PC(sp^3)P bi functional catalysts for additive-free production of H_2 by dehydrogenation of neat Formic acid: Experimental and theoretical study

Dmitri Gelman*, Shirel Cohen, Veniamin Borin, Igor Schapiro
Institute of Chemistry, The Hebrew University, Edmond Safra Campus, Givat Ram, 91904 Jerusalem, Israel.

Reversible storage of hydrogen in the form of stable and relatively harmless chemical substances such as formic acid (FA) is one of the corner-stones of fossil fuels-free economy. Recently, Ru(III)-PC(sp^3)P (where PC(sp^3)P = modular dibenzobarrelene-based pincer ligand possessing a pendant functional group)[1] complex has been reported as a mild and E-selective catalyst in semihydrogenation of alkynes with stoichiometric neat formic acid. Discovery of the additive-free protocol for dehydrogenation of FA launched further studies aiming at the rational design of highly efficient catalysts for this reaction operating under neutral conditions. We now report the results of our investigation on a series of bifunctionl PC(sp^3)P complexes equipped with different outer-sphere auxiliaries, that allowed to identify an amine-functionalized Ir(III)-PC(sp^3)P complex, as a clean and efficient catalyst for the dehydrogenation of neat FA. The catalyst is suitable for fuel cells applications demonstrating TON up to 5*105 and TOF up to 2*104 h^{-1}. In addition to the practical value of the catalyst, experimental and computational mechanistic studies provide rationale for the design of improved next-generation catalysts.

Audience Take Away:

- Design of new catalysts for waste-free decomposition of FA for applications in fuel-cells
- Design of Ligand-metal cooperating catalysts
- Design of new reaction schemes

Biography

Dima was born (1974) and raised in Chelyabinsk, USSR. He received his BSc degree in chemistry (1996) and his MSc degree in Organic Chemistry (1997) from the Hebrew University working with Prof. Zeev Aizenshtat and Prof. Jochanan Blum. He started his doctoral studies in 1999 under the supervision of Prof. Blum and collaboration with Prof. Schumann (TU Berlin) and graduated in 2002 (with distinction). His thesis dealt with the development of air- and moisture stable organo-aluminum alkylating reagents for organic synthetic applications. In 2002, he joined the group of Prof. Stephen L. Buchwald at the Massachusetts Institute of Technology where he spent two years as a postdoctoral associate. His work at MIT concerned the development of catalytic methods for the construction of carbon-carbon and carbon-phosphorus bonds. In 2005, he returned to the Hebrew University of Jerusalem. Now he is an Associate Professor of Chemistry and the Head of School of Chemistry.

Interfacial novel phenomena on heterogeneous photocatalysis

Hideyuki Okumura, Ph.D.
Kyoto University, Japan

Heterogeneous photocatalysis is a photon-driven reaction process with multiple elementary steps or phenomena at the interphase interface, involving generation and transport of electrons, radicals, atoms and/or molecules. It has found various applications, particularly in the field of environmental remediation, however, further activation of photocatalysis and/or its application in energy field is a challenging task towards a sustainable future society.

In this article, particular focus is placed on interfaces of heterogeneous photocatalytic systems, where various novel phenomena are exhibited as special interfacial behaviors. Two particular topics are selected to exemplify such phenomena.

Novel cocatalytic effects of new-type lanthanide oxychloride LnOCl (Ln=Sm,Nd) photocatalysts mechanically-grafted on BiOCl, which is evaluated by photoremoval of nitric oxide (NO) gas, are first introduced, with special emphasis on microstructural analysis on the interface. A significant cocatalytic effect is only exhibited in highly humid air, where, at the (assumed) steady-state, the maximal NO photoremoval rate is ~5 times more than pure BiOCl, or, 20 times if BiOCl would be the only active photocatalyst of the powder composite. There is a characteristic incubation period prior to activation of the novel behavior. Further, when LnOCl is grafted on TiO2 powder, the NO removal rate in humid air is almost completely eliminated. This is opposite to the case on BiOCl. Since, in dry air condition, there is no large difference between TiO2 and BiOCl, water molecules are essential for the special role of LnOCl. This interesting difference between TiO2 and BiOCl will be discussed, besides the novel photocatalysis mechanism involving interfaces and second, activation challenge of light harvesting by magnetic field is discussed. If a key (rate-determining) step of photocatalysis is controlled by magnetic field, wider environmental applications, as well as energy harvesting, would become possible.

Magnetic field effect (MFE) on homogeneous reaction systems has been relatively well-established, however, MFE research on heterogeneous systems, photocatalysis in particular, is limited, and the mechanism is not agreed-upon. Although several MFE parameters have been found responsible for photocatalytic dye degradation, significant roles of oxygen at/near interface are here emphasized. Molecular oxygen is paramagnetic, and typically involved with photocatalysis through ROSs (reactive oxygen species) generation and reactions. In the volume in close proximate to photocatalyst, electrostatic potential and the corresponding magnetic flux would be perturbed, resulting in net Lorentz force acting on dissolved oxygen (DO), which is responsible for MFE phenomena (OANS model). Short-range-order (SRO) diffusion in the Helmholtz layer just outside photocatalyst would be a key step, and correlated to magnetic adsorption/desorption. Through kinetic forces of friction and form drags, DO would cause fluid convection, as "magnetic" diffusion. Representative MFE features on heterogeneous photocatalysis, directly or indirectly associated with interfacial reaction mechanisms, will be discussed, including significant roles of oxygen and water, in terms of molecular perspectives and surface conditions of photocatalyst.

Audience Take Away:

- Investigating detailed surface state is required to understand or enhance photocatalysis.
- An ambient condition (with H2O, O2 and CO2) is often critical for reproducible data.
- Commonly available magnets could be useful for environmental applications.
- Intriguing intellectual and scientific curiosity towards photo-/magneto- science involving interfaces.

Biography

Hideyuki Okumura is Associate professor in Graduate School of Energy Science, Kyoto University. Member of Catalysis Society of Japan, Magneto-Science Society of Japan, Japanese Photochemistry Association, Japan Society of Applied Physics, Electrochemical Society of Japan, Sigma Xi [Scientific Research Society], and serving as an editorial board member for Scientific Reports (Nature Publishing). He holds B.S. and M.S. from Kyoto University, and Ph.D. from University of Pittsburgh. His professional experience includes fellowships at University of Delaware and Carnegie Mellon University, with 96 original papers, 10 international proceedings, 14 books (chapter contributions) and 11 patent applications (4 granted).

Molecularly imprinted polymers electrochemical sensors: Form macro to micro molecules detection

Rasha Mohamed El Nashar
Chemistry Department, Faculty of Science, Cairo University, Egypt

Molecularly imprinted polymers (MIPs) are synthetic materials with so many applications as recognition elements in many types of electrochemical sensors due to their very unique properties including: high thermal stability, longer shelf stability, reusability besides higher selectivity that is comparable to natural biological receptors.

For a chemical sensor to work, two mechanisms are required: recognition and transduction. MIPs play a wonderful role as recognition receptors in combination with a transducer that transforms the concentration of substrate or the product of interaction of the target material in the electrode matrix into electrical signal that is amplified and further processed.

Molecularly imprinted polymers (MIPs) can be easily Incorporated either on polymeric membrane or within solid matrix to form the active electrode surface allowing the design of electrochemical sensors with very fixable analytical characteristics .Also, Magnetic Molecularly imprinted polymers (MMIP) can be utilized to improve properties of the sensor by offering a simple and fast elution of the template molecules from MMIPs by simply using an external magnetic field.

Many other materials were also combined with MIP to give electrodes of improved analytical performance to fit in different applications, such as nanomaterials such as gold and silver nanoparticles (AuNPs and AgNPs), single-walled and multi walled carbon nanotubes (SWCNTs and MWCNTs). Also, different types of MIPs were applied including, bulk, surface imprinted, hydrogels.

The recent advances in application of MIP as recognition receptors will be discussed in this presentation.

Biography

She is full Professor of Analytical Chemistry, Faculty of Science, Cairo University since 2014 and adjunct professor of analytical Chemistry at Zewail City of Science and Technology, Egypt, besides being a former adjunct professor at School of Science and Engineering in the American University in Cairo. She was on scientific leave from Faculty of Science, Cairo University to Faculty of Pharmacy and Biotechnology, The German University in Cairo, since March 2004 till end of June 2015. Her research interests include, Molecularly imprinted polymers synthesis and different applications including solid phase extraction, sensors and drug delivery systems, nanoparticles synthesis, electrochemical sensors, flow injection analysis and computer assisted HPLC method development. She was awarded the prestigious State incentive award for technological science (basic sciences sector) 2015 from The Egyptian Academy of Science and Technology, besides several travel and research grants from DAAD, TWAS and center of special studies in Alexandria library. She is a member of the board of directors of the Egyptian society of analytical chemistry since 2017.

CONTENTS

SCR of NO with C_3H_6 over iron modified Ag/Al_2O_3 catalysts supported on honeycomb ceramic

Yaxin Su*, Wenyi Deng, Xi Yang
School of Environmental Science and Engineering, Donghua University, Shanghai 201620, China

Ag supported on Al_2O_3 catalyst showed good activity in the SCR of NO by HC agents. The resistance of Ag/Al_2O_3 catalysts to H_2O and SO_2 in the flue gas is a problem. Mg was used to modify the Ag/Al_2O_3 catalyst and the resistance of Ag/Al_2O to SO_2 can improved, but H_2O had a great influence on the reduction of NO by $Ag/Mg/Al_2O_3$, e.g., at 350ºC, the addition of 9% H_2O reduced the conversion of NO by 40% and the conversion of reducing agent C_3H_6 by 10% respectively. The resistance of Ag based catalysts to SO_2 and H_2O remains to be further investigated for HC-SCR of NO.

In this presentation, Ag/Al_2O_3 catalysts supported on honeycomb ceramic were prepared by sol-gel and impregnation methods and modified with Fe to promote the catalytic performance for SCR of NO with C_3H_6 and to improve the resistance to SO_2 and H_2O. The catalytic performance to reduce NO with C_3H_6 was evaluated in a one-dimensional electrically heated temperature programmed ceramic tubular reactor in simulated flue gas atmosphere at 200-700°C. The results show that the NO reduction efficiency on $7.2Fe/1.9Ag/20Al_2O_3/CM$ with C_3H_6 is more than 90% and reaches about 100% at the temperatures of 500ºC and 550ºC respectively. Iron can effectively improve the ability of $Ag/20\ Al_2O_3/CM$ catalysts to resist SO_2 and H_2O in flue gas. When SO_2 and H_2O are 0.02% and 8% in the flue gas, the NO reduction efficiency is almost not influenced on $7.2Fe/1.9Ag/20\ Al_2O_3/CM$ at 500ºC. The 90% NO reduction efficiency is maintained during 6 h without decrease. However, the catalytic activity of $2Ag/20\ Al_2O_3/CM$ without iron modification is strongly influenced by SO_2 and H_2O in the flue gas. The NO reduction efficiency on $Ag/20Al_2O_3/CM$ decreases rapidly from about 70% to 46% and 25% respectively, when the SO_2 and H_2O are 0.02% and 8% in the flue gas. The results of XRD and SEM of the catalyst show that $AgFeO_2$ and Fe^{3+} are formed in the $7.2Fe/1.9Ag/20\ Al_2O_3/CM$ catalyst after the modification by iron, and the surface of the catalyst become loose and porous, forming Fe_3O_4-based needle-like and flaky crystals. H_2-TPR results show that $7.2Fe/1.9Ag/20\ Al_2O_3/CM$ has better reduction properties than $Ag/20Al_2O_3/CM$ in the wider temperature range. Pyridine adsorption Infrared Spectroscopy (Py-FTIR) experimental results show that Fe increases the Lewis acid sites in the catalyst surface.

Audience Take Away:

- The presentation provides the audience a new method to prepare the effective catalysts which could be applied to the selective catalytic reduction of NO with hydrocarbon fuels. The resistance to SO_2 and H_2O in the flue gas is greatly improved for practical use. The scientific aspects related to the catalytic reactivity are discussed with characterization results.

Biography

Yaxin Su received his BS of Exploring Engineering from China University of Geosciences in 1994, MS of Mechanical Engineering with a focus on heat transfer from National Huaqiao University, China, in 1997 and PhD of Power Engineering and Thermophysics with a focus on combustion from Zhejiang University, China, in 2000. He worked in the Department of Chemical Engineering, University of Mississippi, USA as a visiting professor during 2006-2007. He is currently a professor in the School of Environmental Science and Engineering, Donghua University, China. He was the Chair of the Department of Built Environment and Energy Engineering during 2006-2009 and also was the course director and coordinator of the joint MS program of Sustainable Energy Technology between Donghua University and the University of Nottingham, UK during 2006-2009. Dr Su has been involved in heat transfer, gas-solid suspension flow and separation, thermo-chemical conversion of solid fuels, such as pyrolysis and combustion of coal, biomass and waste sludge, pollutant emission control, such as NOx reduction, CO2 capture, etc. He has published 3 academic books and 2 textbooks, more than 100 journal articles and 50 international conference papers.

Two-step water splitting under visible light by using Polyoxometalate as shuttle redox mediator

Osamu Tomita*, Hiroki Naito, Kohei Tsuji, Akinobu Nakada Ph. D., Masanobu Higashi, Ph. D., Ryu Abe, Ph. D.
Kyoto University, Japan

Water splitting systems based on two-step photoexcitation, so-called Z-scheme systems, have recently been developed and proven as a promising approach to harvesting a wider range of visible light, because the water splitting reaction is separated into two parts, i.e., H^{2-} and O^{2-}evolving systems. Although the introduction of Z- scheme systems enables us to employ various visible-light responsive photocatalysts, the choice of redox has been limited to simple ion couples such as IO^{3-}/I^- and Fe^{3+}/Fe^{2+}. This is mainly due to the problems with mismatching redox potentials and/or irreversibility presented by other materials. The development of redox couples with appropriate redox potentials and sufficient reversibility under mild pH conditions is thus required in order to achieve highly efficient Z-scheme systems.

Here, we have paid attention to the use of transition metal-substituted-polyoxometalates, most of which are known to exhibit reversible redox behavior derived from valence differences between the incorporated transition metals, as effective shuttle redox mediators. We have recently reported a new Z-scheme water splitting system using a polyoxometalate (POM) as a redox mediator; the use of a Mn-substituted silicotungstate or Mo-substituted one ($K_6[SiW_{11}O_{39}MnII(H_2O)]$ or $K_4[SiW_{11}O_{40}MoVI]$, denoted as $SiW_{11}Mn$ and $SiW_{11}Mo$, respectively) with appropriate photocatalysts enabled a stoichiometric evolution of H_2 and O_2 under visible light. In the present study, V-substituted silicotungstate ($K_5[SiW_{11}O_{40}V^V]$, denoted as $SiW_{11}V)_6$ was prepared and employed as redox mediator to pursue the availability of POM. The $SiW_{11}V^V/SiW_{11}V^{IV}$ was confirmed to function as electron donor in H_2-evolution system or as electron acceptor in O2-evolution system. The $SiW_{11}V^V/SiW_{11}V^{IV}$ was revealed function as effective shuttle redox mediator between the two photocatalysts under visible light irradiation.

Audience Take Away:

- This presentation will introduce the one of the strategies to solve a problem in photocatalytic water splitting. After taking this presentation, they will be able to understand the general problems in water splitting by using photocatalyst powder samples, two-step water splitting in particular. Two-step water splitting by using polyoxometalate as new type shuttle redox mediator will be introduced. They will be able to think about the design of photocatalysts, and the preparation of efficient redox mediator.
- To find and employ the advantage of each material, it will solve the problem and accelerate the research in some cases. I hope that the knowledge related to present topic that is the use of suitable redox behavior of polyoxometalate material will expand the various research containing other field.

Biography

Osamu Tomita received his BS (2006) from Tokyo University of Science, and his MS (2009) and PhD (2012) from Hokkaido University. He then worked as a postdoctoral fellow (2012–2016) at Kyoto University. He is currently an assistant professor (2017–) at Kyoto University. His research interests are photocatalytic water splitting and photocatalytic selective oxidation of organic compounds.

Selectivity controlled with transient operation

Javier Fernandez-Garcia[1]*, V. Matveeva[3], N. Cherkasov[2], E.M. Sulman[3], E.V. Rebrov[2,3]
[1]School of Chemical and Process Engineering, University of Leeds, Leeds, LS2 9DT, UK
[2]School of Engineering, University of Warwick, Coventry CV4 7AL, UK
[3]Department of Biotechnology and Chemistry, Tver State Technical University, Tver 170026, Russia

Transient operation has been previously considered in many industrial processes where either heat recovery or production rate can be considerably improved as compared to steady-state operation. The effect of periodic temperature oscillations have been studied in the hydrogenation and isomerization of D-glucose over a supported Ru-catalyst in a micro trickle bed reactor. It was found that the preferred reaction pathway depends on the frequency of periodic temperature oscillations. The catalyst based on ruthenium nanoparticle supported over hypercrosslinked polystyrene was tested in the reaction of hydrogenation/isomerization of glucose and maltose under radiofrequency heating in a continuous flow fixed bed reactor. The catalytic activity and selectivity were investigated under the steady-state and transient operation reactor modes. The transient operation of periodic temperature oscillations with a low amplitude of 14°C showed a dramatic change in the reaction pathway altering the preferential reaction from hydrogenation to isomerization for both substrates studied. The period of temperature oscillations affects the hydrogen coverage which can determine the main reaction which takes place. The data shows that the transient operation mode could have a high impact on biorefinery because fructose is one of the main feedstocks for 5-hydroxymethylfurfural and other valuable compounds in the field. Moreover, the work demonstrates that a concept of a superior product selectivity achieved by introducing transient operation, which can likely be applied to other reaction classes and processes.

Audience Take Away:

- This presentation could boost collaborations as people would like to study the transient effect on their reactions. They will learn how selectivity could be controlled with this approach, so this could be a breakthrough in reaction engineering.
- This presentation will show a possible new technology for parallel reactions as desired products could be obtained considering parameters of transient operation. This transient operation is a new approach which could mean controlled selectivity for biorefinery, pharmacy and fine chemistry.
- Possible academics and industries could be interested in testing their catalysts with this approach. Strong collaborations could be developed and discussed.
- This can have an impact on pharmacy, fine chemistry and biorefinery.
- It will provide a much wider variety and possibilities for desired products in catalytic reactions.

Biography

Javier Fernandez-Garcia studied his bachelor (2002-2007) and master's degree (2010-2011) in Spain. He worked in industry from 2007 to 2014 in companies such as Saint-Gobain, XSTRATA, Biogas Fuel Cell and HUNOSA. He completed his PhD at University of Oviedo (2011-2014). After that he worked as a Research Fellow at University of Warwick from 2014 to 2016. Then he developed research activities in Stoli Catalysts Ltd (Spin-out Company) and he was finally appointed as Lecturer in Chemical Engineering at University of Leeds in 2017.

magnus
Group

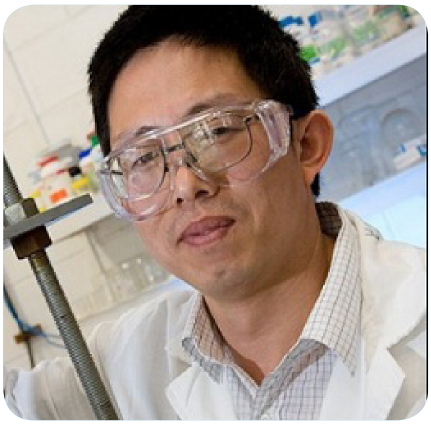
DAY 3

KEYNOTE FORUM

2nd Global Conference on

Catalysis, Chemical Engineering & Technology

September 13-15, 2018
Rome, Italy



Biography

Prof Zhu's research interests exist in advanced catalysis, gas/liquid adsorption and separation, direct carbon fuel cells and solid oxide fuel cells. His publications include one edited book, 8 book chapters, and over 230 journal papers. He holds 7 patents, 3 patents have been licensed to the industrial sponsor. He has raised a total research funding from government and industries in excess of $20 million. He is the recipient of a number of awards, including RK Murphy Medal 2013, Freehills Award IChemE 2011, 2nd place Innovator of the Year Award Global IChemE 2011, the University of Queensland (UQ) Foundation Research Excellence Award in 2007.

Novel Perovskite catalysts for solid oxide fuel cells and water splitting

Zhonghua (John) Zhu, Ph.D.

The University of Queensland, Australia

Solid oxide fuel cells (SOFCs) can effectively convert the chemical energy of fuels into electricity at an efficiency up to 60%. They typically operate at high temperature (800-1000°C) resulting in high costs, materials compatibility and durability challenges. Developing SOFCs that can work at intermediate temperature (500-750 °C) has thus been attracting considerable attentions. The performance of the cathode is the largest hurdle to the full realization of low temperature SOFCs. In the first part of this talk, we will introduce our recent studies on novel perovskite catalysts for highly efficient oxygen reduction reaction in SOFCs. Development of highly active and cost-effective electrocatalysts is central to the large-scale electrolysis of water for hydrogen production. Perovskite oxides are also found to be a group of promising candidates to lower the oxygen evolution reaction (OER) barriers in water splitting, and further improvement of their activity and durability are necessitated. In the second part, we will introduce our recent work on perovskite materials as high performance electrocatalysts in water splitting for hydrogen generation, which actually provides clean fuel for SOFCs.

Audience Take Away:

- Perovskite materials are becoming more and more popular, particularly in clean energy and environmental research areas. From this talk, the audience can learn how to synthesize nanostructured perovskite catalysts, and how to improve their catalytic activity and how to control the thermal and structural stability
- The audience from universities or research institute could use the perovskite materials in their own areas either as catalysts or sensor materials after this talk.
- The audience from industry could also use the perovskite materials as highly efficient and economic catalysts to replace the more expensive catalysts in practice.
- This talk covers two applications: solid oxide fuel cells and hydrogen generation, the first application needs relatively high temperature (say 500-750 oC), while the second application works at room temperature. This talk thus provides a good example on how the same type of perovskite catalysts can work at both high temperature and low temperature. This means that the audience/researchers could explore more applications for perovskite materials.

Biography

Pascal Granger (1964) is professor at the University of Lille, member of the French Chemical Society. His research work is focused on reaction mechanisms and kinetics of catalytic reactions in post-combustion catalysis and catalytic DeNOx and DeN2O abatement processes. He developed the use of perovskite type structures for substituting critical materials such as PGM. He is co-editor of two Wiley Books dedicated to perovskite materials (2015) one book series entitled 'Past and Present in DeNOx catalysis' (2007). He is author and co-author of more than 125 regular articles in peer-reviewed international journals, 6 book chapters, one monography and obtained a Lecture Prize during the International ICEC meeting in Lyon awarded by the Catalysis Division of the French Chemical Society.

Kinetics in heterogeneous catalysis for DeNO$_x$ reactions: How to relate catalytic to surface properties

Pascal Granger, Ph.D.
University of Lille, France

Kinetics for DeNOx reactions in three-way or lean conditions has been the subject of a huge number of investigations over mixed metal oxides and supported metallic catalysts, i.e., Platinum Group Metal. The complexity of these studies is usually related to the involvement of the support and especially the metal/support interface. According to the strength of such interactions, between nano-sized particles and the support materials, the size and the morphology of those metallic particles can be significantly altered inducing modifications in the kinetic behavior typically for structure-sensitive reactions. Some illustrations will be given through the kinetics of the reduction of NO to nitrogen in three-way near stoichiometric conditions and in lean conditions on mixed metal oxides showing the participation of different reaction intermediates. Correlations between kinetic parameters and surface properties will be tentatively established and discussed.

The second part will be dedicated to the role played by the metal/support interface visualized through Temporal Analysis of Products. Fresh and aged Natural Gas Vehicle Catalysts were analyzed from single methane and NO. Results will be discussed in order to identify the most prominent elementary steps governing the catalytic properties on fresh and aged samples.

Audience Take Away:

- The content of this presentation will highlight the difficult problem to relate surface properties of heterogeneous catalysts to their intrinsic catalytic properties and possible evolution under running conditions due to their instability. Selected examples for environmental catalysis will illustrate the complexity in defining the composition of active sites.

CONTENTS

Valorization of chloromethane wastes to valuable hydrocarbons by hydrodechlorination with supported metal nanoparticles catalysts

Luisa María Gómez Sainero, Ph.D.
Universidad Autónoma de Madrid, Spain

Biography

Lecturer in Chemical Engineering at the Autónoma University of Madrid. Previous positions as researcher at the University of Edimburgh (Marie Curie Fellowship), Catalysis Institute (Spanish Research Council) and Erkimia S.A. company. Ph.D. in Chemical Engineering by the Complutense University of Madrid (1997). Principal Investigator of several projects funded by the Spanish Government focused on the treatment of chlorinated organic wastes by gas-phase hydrodechlorination. Her research interests are in the area of heterogeneous catalysis, chemical reaction, H2 production and environmental engineering. She is author of 40 publications, 3 patents and 78 contributions to conferences. Departmental coordinator for International Exchange Programs.

Chloromethanes constitute very dangerous waste products from many industrial processes. Despite their harmful effects, and because of their particular physical and chemical properties, some of them like chloroform (TCM) and dichloromethane (DCM) are still widely used in industry, and consequently large amounts are released in residual effluents through liquid and gas streams. There are several techniques available for their removal; however, their reuse for the production of valuable hydrocarbons would be more interesting. Olefins are currently one of the main building-blocks for petrochemical industry, and ethane and propane constitute very important petrochemical feedstocks for their synthesis. In this study, the valorization of chloroform (CLF) by gas-phase catalytic hydrodechlorination (HDC) with several carbon supported metal catalysts is presented, in order to maximize the selectivity to ethane and/or propane. The influence of the metal selected, support, preparation and operating conditions in the physico-chemical properties of the catalysts and their performance in the process in terms of activity and selectivity was investigated. The catalysts prepared include Pd, Pt, Rh and Ru supported on a commercial activated carbon; Pd supported on several carbons prepared by chemical activation of lignin with different activating agents, like H3PO4, FeCl3 and NaOH; and Pd supported on carbon nanofibers. All the catalysts were prepared by the incipient wetness impregnation method from metal salts, with a metal content of 1wt%. The catalysts were fully characterized by N2 adsorption-desorption at -196 °C and CO2 adsorption at 0 °C isotherms, TPR, NH3-TDP, XRD, XPS and TEM. The HDC experiments were performed in a continuous flow reaction system containing a quartz fixed bed micro-reactor (CTCM= 1000 ppm, H2/DCM (molar) = 100, τ = 0.8 kg_{cat}.h.mol-1 , T= 75-300 oC). Prior to reaction, the catalysts were reduced "in situ" under a H2 flow (50 Ncm3•min-1) at 250°C for 2 h. Pd showed the best performance when compared to the other metals , which can be attributed to the formation of more stable intermediates and/or the lower desorption energies of products, in accordance to previous studies. Pd catalysts were found to be very efficient for the formation of C2+C3 hydrocarbons, with TCM conversions near 100% and selectivities to those hydrocarbons up to 80%. Pd is present in the catalysts surface in zero-valent (Pd0) and electro-deficient (Pdn+) state, with different proportions depending on the catalyst. Mean metal particle sizes in the order of 2-14 nm were obtained. Selectivity to C2+C3 hydrocarbons is favoured by increasing Pdn+/Pd0 ratio and the basicity of the catalyst surface. The intrinsic activity of the catalysts (TOF) increases with metal particle size between the range explored.

CONTENTS

Audience Take Away:

- Society moves toward a circular economy. Recycling of chlorinated wastes to obtain valuable hydrocarbons brings many benefits when compared to other conventional treatment technologies.
- In addition, chloromethanes could be used as intermediates to obtain building-blocks products for the petrochemical industry by catalytic hydrodechlorination. This process could become an alternative to overcome the problems associated to the use of fossil fuels as row materials for this industry and to the high endothermicity of methane reforming process. Choloromethanes can be produced by conventional technologies from renewable raw materials.
- In this study new catalysts were developed to reach the objectives proposed, and practical and scientific aspects of the catalyst and process are discussed in order to maximize the yield to the desired products. It includes the employment of a wide diversity of characterization techniques, in order to determine the physico-chemical properties of the catalysts, which directly influence their catalytic properties.

CONTENTS

Biography

Valérie Meille received her PhD in 1997 from University of Lyon, in the field of kinetics and catalysis. In 1998, she obtained a CNRS permanent position in a Catalytic process engineering laboratory, in Lyon. In 2007, she received the Habilitation from University of Lyon. Her main research field concerns the coating of solid catalysts on structured reactors, but she is also involved in many other research activities of the LGPC lab, like reaction kinetics, catalytic hydrogenation and hydrosilylation, G/L/S reactor characterization.

Modified Mahoney-Robinson reactor using a static catalytic foam characterization and catalytic applications

Valérie Meille, Ph.D.

LGPC-University of Lyon, France

A stirred Mahoney-Robinson reactor has been modified by replacing its basket (usually filled with catalytic beads or extrudates) by a coated solid foam of the same external dimensions (hollow cylinder). Foams were either made of polyurethane or of stainless steel and Pd/C and Pd/alumina catalysts were coated at their surface.

The new reactor was first characterized in terms of G/L and L/S mass transfer. The batch absorption of hydrogen and the measurement of alpha-methylstyrene hydrogenation rate on Pd/alumina were used to evaluate G/L and L/S mass transfer coefficients. The foam showed slightly better performances than the reference bead-basket. However the productivity of the foams was up to 5 times higher than the bead bed due to specific area differences.

Stainless steel foams coated with Pd/C were used to catalyze nitrobenzene hydrogenation. Different sources of carbon were used for the coating (carbon black, activated carbon, carbon nanotubes (MWCNT)). Pd/MWCNT outperformed other coated Pd/C catalysts once coated. The sintering during the thermal treatment of the coating was less severe for this support. During the nitrobenzene hydrogenation, a catalyst deactivation was observed. The in situ electrochemical regeneration of spent Pd/C/foam catalysts was investigated. Its efficiency was assessed by monitoring the catalyst activity versus cumulative turnover number (TON). The results showed that the catalyst activity was fully recovered after regeneration and that the catalyst had the same deactivation rate after several reaction/regeneration cycles. This result validates the potential use of such modified Mahoney-Robinson reactor as a continuous stirred-tank reactor.

Finally, cylindrical polyurethane foams cut to fit a Mahoney-Robinson reactor were used. Polyurethane could bring several advantages compared to stainless steel, such as an easy availability, a low price, an easy handling and a better uniformity than metallic foams which generally suffered from successive process operations. To allow the coating of polyurethane foams (PUF) by a Pd/alumina catalytic layer we report the use of polydopamine (PDA) as a primer. Cylindrical polyurethane foams were first coated with a PDA layer and then successfully coated with a Pd/alumina powder catalyst. The coated foam was used in successive batch hydrogenations of alpha-methylstyrene. 6 successive runs were possible, reaching a total turnover number of 36000 mol(cumene)/mol(Pd)). The activity of the catalyst was still high at the end of the 6th run (more than half the activity of the fresh catalyst). No palladium leaching was noticed. The use of coated polyurethane foams in catalytic reactions is thus possible, whereas limited to low temperature reactions due to the thermal stability of polyurethane. Moreover, as the coating is very thin, such a configuration is recommended for very fast, mass-transfer limited reactions.

Audience Take Away:

- A very mass-transfer efficient reactor is proposed and can be used to replace the Mahoney-Robinson reactor
- It can be used as a continuous stirred-tank reactor, with the catalyst coated on the surface of the foam, without leaching, and with the possibility to regenerate the catalytic activity after deactivation.
- The coating of the foams is easily obtained by dip-coating in a suspension of the catalyst.
- Even polyurethane foams can be used, for fast reactions at low temperature.

Applications of visible light-driven photocatalysts to photocatalytic degradation and PEC water splitting

Byeong-Kyu Lee, Ph.D.

University of Ulsan, Republic of Korea

There have been many developed photocatalysts that could be applicable for pollutant removal and energy generation. The first part of the presentation can provide principle of photocatalysis, limitation of TiO_2 photocatalysts, increasing solar energy utilization, modification methods to build visible light-driven photocatalyst, including metal and non-metal doping, using sensitizer and another semi-conductor, etc. The presentation also deals with immobilization methods of photocatalysts using porous materials and chemical reactions, VOCs removal methods using visible light-driven photocatalysts, bioaerosol removal results, and CO_2 conversion to solar fuels and methanol, and other environmental applications. The last part of the presentation deals with principle of photoelctrochemical (PEC) water splitting, applications in photodegradation and PEC water splitting of modified bismuth vanadate with structural transformation and reduced graphene oxide (rGO).

Audience Take Away:

- The audience would learn how to develop visible light-driven photocatalysts
- The audience would get exposed to some application ideas of visible light-driven photocatalysts in organics and VOCs removal in air, bioaerosol removal, and CO2 solar fuel conversion
- The audience would get some ideas of modifying photocatalysts for improving organics removal from aqueous media and PEC water splitting for H2 production or renewable energy.

Biography

Byeong-Kyu Lee is a Distinguished Professor of Civil and Environmental Engineering at the University of Ulsan (UOU), Korea. Prof. Lee is the Director of Brain Korea 21 and got his MS and Ph.D. degrees from UMASS and joined as a visiting scientist at Harvard University and UMN. He received a Service Merit Medal of Korea from Korean Government and an Outstanding Professor Award from AWMA. He has published over 200 peer reviewed scientific journal papers, 15 book chapters, 16 patents, and over 300 conference papers. Prof. Lee's current research interests include visible photocatalytic treatments of organics/VOCs, photocatalytic CO2 conversion into solar fuels, photoelectrochemical H2 production, and CO2 sequestration using nano zeolites and nanocomposites.

Biography

Juha Lehtonen (Dr. Tech. in Chemical Engineering) is a Research Professor of Bioenergy and Thermochemical Processes at VTT Technical Research Centre of Finland. His research is focusing on catalytic and thermochemical conversion of biomass and carbon dioxide, heterogeneous catalysis, reaction engineering and renewable fuels and chemicals. He is an author or co-author of over 70 peer-reviewed publications. He obtained his doctoral degree (chemical reaction engineering) at Åbo Akademi University, Finland. His thesis was awarded as a best doctoral thesis in the field of chemical engineering in 1996 - 1997 in Finland. He has a long career in industrial research organizations as a specialist of chemical reaction engineering, catalysis and development of biofuels processes. He has also experience of many managerial positions in industrial R&D organizations. Before moving to VTT, prof. Lehtonen worked at Aalto University, Finland as a professor of Industrial Chemistry.

Catalysis for biomass conversion to traffic fuel compounds

Juha Lehtonen, Ph.D.

VTT Technical Research Centre of Finland Ltd., Finland

Lignocellulosic biomass is the most abundant raw material to produce sustainable advanced traffic fuels. However, conversion of solid biomass to high quality liquid fuels has turned out to be challenging due to heterogeneous nature of biomass. Lignocellulosic biomass can be converted into liquid fuels by applying thermochemical methods such as gasification or fast pyrolysis and by further upgrading the intermediates. Alternatively, biomass can be fractionated and the constituents (cellulose, hemicellulose, lignin) can be upgraded separately to liquid fuels by chemical or biochemical conversion. In all of these routes, except in the biochemical conversion, heterogeneous catalysis is in key role. In gasification route, efficient catalysts are needed for gas cleaning and synthesis gas upgrading to liquid products. Heterogeneous acid catalyst can be applied for fast pyrolysis (catalytic fast pyrolysis) to improve the properties of bio oil or they can be used for bio oil upgrading either to remove the oxygen by hydrodeoxygenation (HDO) or to crack the bio oil by acidic zeolites e.g. in oil refinery FCC units.

Both sugar fractions (cellulose and hemicellulose) and lignin can be upgraded by heterogeneous catalysts. Sugars can be converted to HMF (celluilose) or furfural (hemicellulose) by heterogeneous acid catalysts and further upgraded to dimetylfuran (DMF) and 2-methylfuran (DMF) by catalytic hydrotreatment using advanced metal catalysts, respectively. Both, 2-MF and DMF are promising new bio-based gasoline components with good fuel properties.

Lignin is a challenging raw material for the upgrading due to it's high reactivity. On the other hand, it is an attractive source of aromatic hydrocarbons to be used for the applications where aromatics are needed such as jet fuels. Lignin can be depolymerized by solvolysis or hydrogenolysis where many different supported metal catalysts have been studied. In solvolysis, liquid hydrogen donors such as ethanol are used whereas in hydrogenolysis, molecular hydrogen is provided to the reactor. The main role of hydrogen is to prevent undesired re-condensation reactions and the depolymerization mainly takes place by thermal or catalytic cracking. Another strategy to depolymerize lignin is to apply fast or catalytic fast pyrolysis. In both cases, depolymerized lignin can be further upgraded by hydrodeoxygenation to remove remaining oxygen.

Audience Take Away:

- Lignocellulosic biomass can be upgraded to advanced traffic fuels by many different routes (thermochemical, catalytic, biochemical)
- Heterogeneous catalysis is involved in most of these routes and is in key role when developing more efficient biomass conversion processes
- Development of more efficient heterogeneous catalysts is still needed to commercialize the processes from biomass to advanced traffic fuels
- VTT is able to develop new advanced heterogeneous catalysts and new processes to upgrade biomass to traffic fuels

magnus
Group

DAY 3

SPEAKERS

2nd Global Conference on

Catalysis, Chemical Engineering & Technology

September 13-15, 2018
Rome, Italy

Nanoparticle beam deposition: A novel route to the creation of heterogeneous catalysts

Richard E. Palmer
Nanomaterials Lab, Swansea University, UK

Size-selected nanoparticles (atomic clusters) represent a new class of model systems for catalysis research. However very rarely have their structures been obtained from direct experimental measurements. The availability of aberration-corrected HAADF STEM is transforming our approach to this s**tructure challenge**. I will address the atomic structures of size-selected Au clusters, deposited onto standard carbon TEM supports from a mass-selected cluster beam source. Specific examples considered are the “magic number clusters” Au20, Au55, Au309, Au561, and Au923. The results expose, for example, the metastability of frequently observed structures, the nature of equilibrium amongst competing isomers, and the cluster surface and core melting points as a function of size. The cluster beam approach is applicable to more complex nanoparticles too, such as oxides and sulphides.

A second major challenge is to translate the beautiful physics and chemistry of clusters into applications, notably catalysis. Compared with the powerful colloidal route, the nanocluster beam approach involves no ligands, particles can be size selected by amass filter, and particles containing challenging combinations of metals can readily be produced. However, the cluster approach has been held back by extremely low rates of particle production, only 1 microgram per hour, sufficient for surface science studies but well below what is desirable even for research-level realistic reaction studies. In an effort to address this **scale-up challenge**, I will discuss the development of a new kind of nanoparticle source, the “Matrix Assembly Cluster Source” (MACS). The results suggest cluster beam yields of grams per hour may ultimately be feasible; mg scale has been demonstrated. Some practical catalysis applications, both gas and liquid phase, will be presented, showing attractive activities and especially selectivities.

Audience Take Away:

- A new method to generate precision catalyst particles in the sub-5nm range on powder surfaces.
- Control of size, and of shape via nanoparticle impact energy.
- Control of composition in binary and complex systems.
- No solvents, + no effluents = green manufacturing.
- Results to date show excellent turnover and selectivity in fine chemicals and electrocatalysis.

Biography

Richard Palmer runs the Nanomaterials Lab in the College of Engineering of Swansea University, Wales, and is Professor in the School of Physics of Nanjing University, China. His research is currently focused on Nanoparticle Beam Deposition, including scale-up and atomic structure/dynamics with applications including catalysis, biomedicine and advanced materials for IT. At Cambridge (1980-1994) Richard was awarded an MA and PhD and held 1851, Clare College and Royal Society Fellowships. At Birmingham (1994 -2017) he founded the UK's first nanoscience centre. Awards include: IOP Boys Medal, Honorary Doctorate from Hasselt University, BVC Yarwood Medal and an EPSRC Senior Fellowship. He is a Fellow of the IOP, RSC and LSW. He has published ~400 papers with h index 53 and ~20 families of patent applications. Spin-off companies include Inanovate and Irresistible Materials. He is the Editor-in-Chief of Advances in Physics: X (Taylor and Francis) and Book Series Editor of ‘Frontiers of Nanoscience’.

CONTENTS

Kinetic modelling of glycerol oxidation on metallic supported catalysts

José Diaz[1], Ph.D., Elżbieta Skrzyńska[2], Soraya Zaid[3], Ph.D., Ayman El-Roz[3], Michael Capron[3], Jean-Sébastien Girardon[3], Franck Dumeignil[3], Helena Ocana[4], Dominique Richard[5], Ph.D., Myriam Frey[5], Ph.D., Pascal Fongarland[6*], Ph.D.

[1]LGPC, UCLM
[2]Cracow University of technology, Poland
[3]UCCS, University of Lille, France
[4]LGPC, France
[5]CNRS, LGPC, France
[6]LGPC, University of Lyon, France

Due to the growing interest in the use of renewable energy sources, glycerol has become an important bio-building block. Catalytic oxidation of glycerol in liquid phase lead to add-value products such as glyceric, glycolic or tartronic acids, which can be used in food, cosmetics, and textile industries. Regarding the catalysts, Au and Pt have been proven to be good active phases: the first one is stable in the reaction media, whereas the second one is very active and selective to glyceric and tartonic acids. On the other hand, the use of Ag has been seldom studied, but it has some advantages: it is selective to C-C cleavage products, and much cheaper than Pt and Au. The aim of this work is to give a quantitative comparison of Au, Pt and Ag as active phases in glycerol oxidation using a kinetic modelling including if necessary deactivation. Based on a simplify reaction scheme, we can determine the effect of the metal nature on selectivity. Inhibition of glycerol and products have been investigated through a pseudo Hougen-Watson-Langmuir-Hinshelwood approach indicating that some acidic species could strongly limited the reaction in line with recent works dealing with DFT calculations. Finally, we have also contributed to try to better understand glyceraldehyde formation in neutral/acidic conditions with Pt catalysts where a quasi-irreversible inhibition similar to a deactivation behavior, has been identified increasing when pH is decreasing. Current work is focused on the determination of a detailed mechanism to build a more accurate kinetic model specially to incorporate the effect of Ph in kinetic constants.

Audience Take Away:

- A demonstration of the utility to develop kinetic modelling even with a very simple mechanism to quantify the effect of catalyst on selectivity (chemical engineering approach useful even for understanding issues)
- A better understanding of glycerol oxidation and the effect of pH
- Some issues for the process development for oxidation reactions without adding inorganic base

Biography

The presenting author, Pascal Fongarland, has defended his Ph.D in 2003 on kinetic measurements of HDS reaction. He got an assistant professor position in 2005 at “Laboratoire de Catalyse de Lille/Ecole Centrale de Lille” focusing his research on Fischer-Tropsch reaction (kinetic and catalytic reactor issues). In 2011, he reached “Université Claude-Bernard Lyon 1” as full professor and was member of IRCELYON focusing of the development of catalytic processes related to the biomass conversion. More recently in 2016, he was designed as director of “Laboratoire de Génie des Procédés Catalytiques.”

Demonstration of a Kilo-scale continuous hydrogenation

Eneritz Fernandez-Puertas*, Lee Edwards, Katherine Wheelhouse, Glynn Williams
GlaxoSmithKline, Medicines Research Centre, Gunnels Wood Road, Stevenage, Hertfordshire SG1 2NY, UK

In the pharmaceutical industry catalytic hydrogenation reactions are normally conducted in batch mode. However, these type of reactions tend to be benefit by continuous processing, as the catalytic continuous reactors offer a high catalyst loading, high pressure operation and enhanced mass transfer. This presentation will show the steps and methodology followed to develop a continuous hydrogenation process. The selection of catalyst was performed based on the chemical and physical properties. A series of batch and flow experiments were performed in order to get an understanding on the reaction mechanism and select the appropriate operating conditions to maximise product yield and minimise formation of by-products. The process was successfully demonstrated in a lab scale catalytic reactor, processing 1.2 kg of substrate and showing a consistent performance over 19 hours of operation. The lab scale process demonstration and the process understanding generated was then used to advise scale-up.

Audience Take Away:

- From this talk the audience will get an overview of the steps that can be followed to develop and optimise a continuous hydrogenation.
- The audience will get an understanding on how the catalyst selection is performed for a trickle bed reactor based on the physical and chemical properties.
- From this talk the audience will get an understanding on the parameters that need to be controlled to ensure a successful scale-up.

Biography

Eneritz graduated from a 5-year Chemical Engineering degree from the University of the Basque Country. She then moved to the United Kingdom to study an MSc degree in Advanced Chemical Engineering with Process Systems Engineering at Imperial College London, followed by a PhD in Chemical Engineering at the same university. Eneritz has been working on the implementation of continuous processes within the manufacture of active pharmaceutical ingredients at GlaxoSmithKline since 2016.

Designing "Nanogold-on-carbon" catalysts for green production of Gluconates and Glyphosate

Boris L. Moroz*, Ph.D., Pavel A. Pyrjaev, Oxana P. Taran, Valerii I. Bukhtiyarov
G.K. Boreskov Institute of Catalysis, Novosibirsk 630090, Russia

It is well known that gold particles with a size of several nanometers exhibit a very high catalytic activity and/or unusual selectivity in numerous redox reactions. Different procedures have been developed for producing the catalysts containing Au nanoparticles on oxide supports, their catalytic properties being tested in detail. Meanwhile, for many potential applications of gold catalysts carbons would be preferable support materials because of their outstanding qualities. However, easy- to-use methods for synthesis of uniform-sized small Au particles on carbon materials are still lacking. Our report will present the outcomes of our efforts to develop a practical technique for preparation of the finely dispersed Au/C catalysts, which is based on the use of a cationic Au(III) tetraammine complex easily synthesized from HAuCl4 as a precursor of catalytically active component. The results of XRD, TEM, XPS and XANES/EXAFS characterization of this catalysts will be discussed, as well as the data of their testing for the aqueous-phase aerobic oxidation of glucose to gluconates, which are widely used biocompatible and biodegradable chemicals, and for oxidative dealkylation of N-alkyl derivatives of glyphosate. The latter represents the final stage of the eco-friendly ("atom-efficient") method for production of glyphosate which is the most-used systemic herbicide in the world.

Study of the Au/C catalysts in aerobic oxidation of glucose in the presence of NaOH/H2O at 60ºC and pH ca. 9 showed their outstanding catalytic performance that allows producing Na gluconate with 96-97% selectivity at ca. 95% conversion. The impact of the mass-transfer process on the overall reaction kinetics in dependence on the support pore texture, the mean grain size of the catalyst and penetration depth of gold into the catalyst grain will be considered on the basis of the data obtained. It will be demonstrated that at low glucose/Au molar ratios, when O2 dissolution in the aqueous phase is the rate-determining step of the process, the rate of glucose oxidation over the Au/C catalysts exceeds that over the Au/Al2O3 catalysts, which is attributed to a higher adhesion of the hydrophobic carbon support to the gas–liquid interface facilitating the oxygen mass transfer towards catalytic sites. Addition of palladium to the Au/C composites provides a further increase in the catalytic activity and selectivity due to formation of the alloyed Pd-Au nanoparticles and possibility of "concerted" reaction mechanism.

Finally, we will demonstrate that the Au/C catalysts possess good catalytic activity and selectivity for aqueous-phase oxidative dealkylation of N-isopropyl-N- (phosphonomethyl) glycine to glyphosate at 70ºC and atmospheric pressure with H2O2 as the oxidizing agent (93.1% selectivity at 98.1% conversion in 120 min after the beginning of the catalytic run). The highest yield of glyphosate is provided by nanogold deposited onto the pre-oxidized carbons. Testing other N-substituted glyphosates reveals that both the substrate reactivity and selectivity for glyphosate increase with the electron-donating effect of the substituent at the nitrogen atom. The mechanism of N-IPMG dealkylation with H2O2 over the carbon-supported gold catalysts explaining this pattern and the reason for the promoting effect of surface acidic groups will be presented, as well.

Audience Take Away:

- The presentation that we propose for inclusion in the CAT 2018 programme offers a novel feasible procedure for synthesis of the uniform-sized small (2-5 nm) gold particles on carbon supports based on the "cationic adsorption" method and expands the scope of gold compounds used as the starting materials for preparing the gold-on-carbon catalysts.
- The experimental facts will be provided proving that the use of a gold complex precursor which would be anchored onto the carbon surface via ligand or ion exchange reactions with the surface functional groups rather than to be reduced either by these groups or free electrons of a carbon matrix, can significantly improve dispersion of Au particles formed after treatment of a catalyst precursor with H2.

CONTENTS

- The conducted study on the contribution of mass transfer processes to the overall kinetics of glucose oxidation in the presence of Au/C and Au/Al2O3 catalysts help to clarify the links between catalyst morphology and apparent catalytic activity. In particular, we will demonstrate that the most promising catalysts for the process are those containing small Au nanoparticles (1–5 nm) in an external thin layer (ca. 5□m) of catalyst granules, i.e. with an "egg shell" distribution of gold. It will be also shown that use of hydrophobic materials as the catalysts supports and application of reactors with highly intensive mass transport is preferable, since the reaction rate of aerobic glucose oxidation at low glucose-to-gold ratios (i.e. under industrially relevant conditions) is determined by O2 dissolution in the aqueous phase. We believe that the development of catalyst preparation techniques and tackling the chemical engineering issues, taking into account the reported results, will contribute to the sustainable production of gluconates and gluconic acid on a large scale.
- It will be first reported that nanogold catalysts may possess high catalytic activity and selectivity for oxidative N-dealkylation of N-isopropyl glyphosate (NIPG) that considerably exceeds the performance of Pt catalysts which are conventionally used in this reaction. We would also like to discuss the reaction mechanism and the reason for promoting effect of acidic groups on the carbon support surface. The conclusions drawn might be useful for intentional design of catalysts and catalytic processes of NIPG dealkylation to glyphosate which represents the largest selling herbicide worldwide.
- Finally, we believe that the report will be of interest to a very wide range of catalytic community members, since the finely dispersed Au/C composites also attractive as catalysts for CO oxidation in air cleaners, breathing apparatuses, fuel cells, gas sensors etc., not only for the liquid-phase oxidation of organic compound.

Biography

Boris Moroz was trained in Chemistry in Tomsk State Unversity (Russia) and then undertook a PhD in Chemistry at Boreskov Institute of Catalysis (BIC) in Novosibirsk, when he designed the bimetallic catalysts for alkene hydroformylation in the group of Prof. V. Likholobov. In 1984, BM was offered a permanent research position in BIC in a laboratory devoted to catalysis by metal complexes. Since 2002, he is a leader of a research team at BIC which developed supported gold-based catalysts for various applications. During this period, he was working as a visiting scientist in the research centers in India, Germany and USA. BM has co-authored about 70 peer-reviewed articles and the International Handbook on Heterogeneous Catalysis (2007). He also teaches at the Novosibirsk State University as an Associate Professor; his teaching curriculum includes Organic Chemistry: An Introductive Course and Inorganic Synthesis. Besides scientific and teaching activities, BM enjoys rock music and jazz, history and traveling.

CONTENTS

Nanoscale platinum particle @ nanostructured carbon materials for catalytic reduction of endocrine-disruptors

Samia Mahouche-Chergui*, Abdallah Oun, Benjamin Carbonnier
Université Paris-Est, ICMPE (UMR 7182), CNRS, UPEC, F- 94320 THIAIS, France

As a new class of functional nanostructures, hairy carbon nanotubes (CNTs) consisting of CNTs-grafted chelatant polymers have attracted considerable attention in designing of metallic nanoparticles platforms. These metal NPs-based nanohybrids exhibit remarkable catalytic activity and recyclability.

In this work we developed a new strategy to prepare functional hairy CNTs for immobilizing nanoscale platinum particles, combining in situ photoinduced SI-ATRP and thiol-yne photo-triggered click reaction. To do this, we have followed a four-step procedure: (i) use of in situ generated diazonium compound to functionalize CNTs by OH-terminated aryl layers; (ii) grafting of bromine ATRP initiator via a nucleophilic substitution reaction, (iii) growing of clickable poly(propargyl methacrylate), PPGM chains from bromine-functionalized CNTs, (iv) grafting of mercaptosuccinic acid via a photoactivated thiol-yne reaction providing chelatant CNT platforms, and (v) in situ generation of platinum NPs on the nanostructured CNTs. The as-platinum nanoparticles decorated CNT-PPGM-SCOOH, served as stable and reusable catalysts for the complete transformation of nitroaromatic endocrine disruptors.

This synthetic approach based on combination of photo-induced SI-ATRP and thiol-yne click chemistry can be used as a general procedure for the controlled design of stable and high-performance novel nanostructured multifunctional platforms.

Biography

Dr Samia Mahouche-Chergui obtained her Master degree in Inorganic Chemistry at Paris Sud University in 2006, and then her PhD in Surface-Interface Chemistry at Paris Diderot-P7 University in 2009. She worked then as a Lecturer/Researcher (ATER) in the same research Group developing a combination of diazonium compounds and click chemistry for the preparation of carbon hybrid materials. After postdoctoral research with Pr. Y. Grohens at the Bretagne Sud University from 2010 to 2012, she joined the East Paris Institute of Chemistry and Materials Science at the University Paris-Est Créteil as an assistant professor. Her research is currently focused on the development of sp2 carbon and clay based-functional hybrid nanostructures for applications including nanofillers, electrochemical sensors, and heterogeneous nanocatalysts.

Study of kinetics and mechanisms of catalytic pyrolysis of biomass components by using linear free energy relationships and TPD-MS

Tetiana Kulik[1]*, Ph.D., B. B. Palianytsia[1], M. Larsson[2], M. Kartel[1]
[1]Chuiko Institute of Surface Chemistry National Academy of Sciences of Ukraine, 17 General Naumov Street, 03164 Kyiv, Ukraine
[2]Stockholm University, AlbaNova University Center, Department of Physics, SE-106 91 Stockholm, Sweden

The conversion of biomass into chemicals and fuels is the most promising avenue being considered by countries to help them reach their renewable energy and feedstock goals and move from hydrocarbon-based chemicals to bio-based chemicals. Non-food biomass is considered to be a feedstock of crucial importance. Currently, the only industrially feasible and "green" technology for conversion of such biomass is heterogeneous catalysis. It is crucial to have a precise understanding of the catalytic transformation mechanisms of main components of biomass on the surfaces of metal oxides.

In this study, we used TPD MS to investigate the pyrolysis of fatty acids on various oxide surfaces. Detailed and targeted kinetic studies for reacting series of fatty acids C2-C18 and triglycerides on the surfaces of nanosized CeO_2, CeO_2/SiO_2, SiO_2, γ-Al_2O_3, Al_2O_3/SiO_2 and TiO_2/SiO_2 have been investigated by the Linear Free Energy Relationships (LFERs) principle and temperature-programmed desorption mass spectrometry. Fourier transform infrared spectroscopy (FTIR) has also been used to investigate the structure of fatty acids complexes on the oxide surfaces. Two reaction pathways of fatty acids conversion were found to be dominant—ketenization to form alkyl ketenes and ketonization to form dialkyl ketones. The kinetic parameters (Tmax, n, E≠, ν0, and dS≠) of ketonization and ketenization were calculated. The first order of ketonization reaction was confirmed by using the Arrhenius Plot method and by investigating the effect of the degree of the surface coverage on the reaction rate. Taft correlation "structure-reactivity" for fatty acids ketonization on the surface of CeO_2/SiO_2 nanocomposites, has been found. Based on these results modified concerted mechanism of the ketonization has been proposed. It was found that the activation energy of ketenization decreases in the order $SiO_2>Al_2O_3>TiO_2/SiO_2>Al_2O_3/SiO_2$, and the activation energy of ketonization decreases in the order $Al_2O_3>CeO_2/SiO_2$. CeO_2 and Al_2O_3/SiO_2 are suitable catalysts for ketonization and ketenization respectively. These catalytic materials provide excellent performance with very low temperature conversions and high selectivities.

Audience Take Away:

- The application of the modified Taft equation (T.V. Kulik, J. Phys. Chem. C 2012, 116, 570 – 580) and the linear free-energy relationships (LFERs) method to the establishment of the catalytic reactions mechanisms will be demonstrated by the example of thermal transformations of the reaction series of fatty acids on the surface of various oxides. The proposed modified Taft equation can be considered a universal equation for studying the kinetics and mechanisms of thermal catalytic reactions.

Biography

Kulik has completed her Ph.D. from Chuiko Institute of Surface Chemistry. She is the Head of Laboratory of the Kinetics and Mechanisms of Chemical Transformations on Solid Surfaces. The main research directions of the laboratory are 1) application of temperature programmed desorption mass spectrometry (TPD MS) to solve problems of surface chemistry and catalysis; 2) heterogeneous catalytic pyrolysis of renewable biomass components for a development of green technologies of synthesis of bio-based chemicals and biofuels. Three Ph.D. theses were defended under her supervision. She has published more than 60 papers in reputed peer-reviewed journals.

Prolong the catalyst life cycle of naphtha catalytic reforming process by optimization of operating conditions

Sorood Zahedi Abghari*, Saied Shokri
Ph.D. of chemical Engineering, Process development and process control Department, Process development Division, Research Institute of Petroleum Industry (RIPI), Tehran, Iran

To lengthen the catalyst life cycle of a Pt-Re/γ-Al_2O_3 catalyst of Naphtha catalytic reforming process and to improve the yield of reformate, an optimization procedure was applied. At first a pilot plant was designed and set up. Based on the industrial operating condition of the process, the operating conditions of the experiments were determined. Then a set of experiments was designed and analyzed based on Central Composite Design (CCD) method. Based on the results of conducted experiments the impact of reactor inlet temperature, feed flow rate and reactor pressure are investigated. To determine the effect of some other operating conditions including chloride injection flow rate and the average boiling point of naphtha feed stock, a wide range of industrial data had been collected in a six-year- operating period. Moreover, a data-driven-model was developed, trained, tested and validated by utilizing the collected information. Also, a rigorous model was developed based on experimental data and retuned with Industrial data. To determine suitable operating condition an evolutionary optimization algorithm was applied. It is concluded that despite the common belief, increasing the inlet temperature of the reactor is not always a suitable way to compensate the deactivation effects of the naphtha catalytic reforming. Indeed, considering certain changes in feed flow rate, reactor inlet temperature, reactor pressure and chloride injection over time is prolonged the catalyst life. Moreover the energy consumption is minimized and the RON of the produced gasoline is maximized. It is also shown that, increasing the chloride injection increases the (C3+C4)/C1 to a maximum point. However, this ratio falls rapidly with higher chloride injection rate. Which decreases the yield of reformate, changes the RVP of produced gasoline and declines the quality of recycle stream which is fed to the reactors. Consequently it deactivates the catalyst. It is also shown that the mean average boiling point of naphtha feed stock have strong effects on RON, production of light hydrocarbons and Yield of reformate.

Audience Take Away:

- The Audiences will be able to develop data driven model and use it to conduct pseudo dynamic optimization of a process. It could be very useful for the researchers or the people who works in the field of process optimization, process debottlenecking and soft sensing in the refinery processes. Since the presentation contains some experimental data, it could be useful for researcher who focuses in the Naphtha catalytic reforming reactors. It also helps engineer who works in the field of product scheduling and production planning of refinery complexes.

Biography

Sorood Zahedi Abghari obtained his PhD of chemical engineering at Tarbiat modares university. He is currently research assistant professor at Research Institute of Petroleum Industry (RIPI) for modeling, simulation and optimization of chemical process. Currently, he is the project manager of designing of an online crude oil blending system. Also, he is the supervisor of six MSc theses. Moreover, he works as the consultant engineer of ODCC Company in the field production planning of Refinery complexes and feasibility study project of different chemical processes.

Selective oxidation of free mono- and oligosaccharides using photocatalysis

Mehdi Omri, Frédéric Sauvage, Matthieu Becuwe, Anne Wadouachi, Gwladys Pourceau*
Laboratoire de Glycochimie, des Antimicrobiens et des Agroressources, UMR CNRS 7378, Amiens, France
Laboratoire de Réactivité et Chimie des Solides, UMR CNRS 7314, Amiens, France

Thanks to their renewability and abundance, the use of carbohydrates as biomass feedstock and their eco-friendly conversion into useful chemicals are becoming increasingly attractive to prepare products capable of replacing petroleum-based chemicals. Sugars are polyfunctional and so, can lead to a wide variety of high-value products such as detergents, pharmaceuticals and cosmetics after chemical modifications. However, usually, glycochemistry does not satisfy the chemistry principles and shows difficulties to be transferred into industrial levels: multi-step protocols and hazardous chemicals are often required. Therefore, the development of novel oxidation methodologies using reusable heterogeneous catalysts and eco-friendly procedure is a very interesting alternative. Heterogeneous photocatalytic transformation constitutes a viable and environmentally friendly procedure since it can be ideally driven only by sunlight absorption. One of the best and most versatile photocatalyst developed so far is the anatase TiO_2, which suffers from several drawbacks such as its large band-gap value of 3.20 eV restricting its absorption to UV light and its poor selectivity. The poor light harvesting can be overcome by the introduction of noble metal nanoparticles such as Au which affords to extend light absorption up to ca. 550 nm thanks to concomitant surface plasmon resonance effect (SPR). In addition, gold NPs in contact with an adequate semi-conductor prolongs the excited-state lifetime of gold as a result of the improved charge separation process. These photocatalytic properties open new perspectives for photo-assisted organic chemistry and for the selective photo-oxidation of organic compounds. We present herein a fast and efficient methodology for the selective photo-oxidation of mono- and oligosaccharides into corresponding sodium aldonates in only 10 minutes under standard incident sunlight irradiation. Three photocatalysts will be compared, namely Au/Al_2O_3, Au/TiO_2 and Au/CeO_2, the latter being the most efficient (TOF > 750 000 h^{-1}) and perfectly selective. The versatility of this methodology will be discussed and the reusability of the photocatalysts demonstrated. We will also discuss the nature of the intermediate species governing the mechanism, thanks to complementary investigations.

Audience Take Away:

- From this talk, the audience will be able to synthesize three kinds of photocatalyst: Au/Al_2O_3, Au/TiO_2 and Au/CeO_2
- Thanks to this methodology, the audience will be able to synthesize in less than 10 min pure oxidized mono- or oligosaccharides
- Thanks to complementary investigations, the audience will be able to understand, in part, the photon-induced charge transfer mechanisms (fundamental research)
- After this talk, the audience from universities or research institute could try to apply this methodology in their own areas (applied research)

Biography

Gwladys Pourceau is an assistant professor of the University of Picardie Jules Verne, Amiens, France. After a Ph.D thesis in Chemistry completed in 2010 at Montpellier (France), she joined the CICBiomaGUNE as a post-doctoral fellow (San Sebastian, Spain) to work on the development of magnetic and/or gold glyconanoparticles. Since 2012, her research activities has been mainly devoted to the development of eco-friendly methodologies to transform carbohydrates. In collaboration with the group, she is developing different approaches amongst nanocatalysis, microwave-assisted synthesis, mechanochemistry and since more recently photocatalysis. All of her scientific activities led to 20 peer-reviewed articles, 6 proceedings, 3 book chapters, 1 patent, 2 patent disclosures, 1 thesis award, and 2 poster awards.

Controlled generation of binary nanoparticles for catalysis research

Maria Chiara Spadaro*[1], Ph.D., Lidia Martinez[2], Ph.D., Hans Fredriksson[3], Ph.D., Jo Humphrey[4], Ph.D., Richard E. Palmer[5], Ph.D.

[1]College of Engineering, Swansea University, United Kingdom
[2]Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigationes Cientifica (CSIC); Rongsheng Cai, M S, College of Engineering, Swansea University, United Kingdom
[3]Laboratory of Physical Chemistry of Surfaces, Eindhoven University of Technology & SynCat@DIFFER, Syngaschem
[4]National Physical Laboratory; Yves Huttel, Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigationes Cientifica (CSIC) , United Kingdom
[5]College of Engineering, Swansea University, United Kingdom

Heterogeneous and electrochemical catalysis is a diverse area of research that finds applications in clean energy technology and the reduction of environmental pollution. Among many metals, the current best catalysts typically rely on critical materials, such as platinum (Pt). As per the EU list of critical raw materials for 20171, Pt needs to be reduced/replaced with abundant materials. Here we present our results on the study of precision nano alloy particles with the ultimate objective of Pt reduction.

Pt-Cu bimetallic clusters have been produced via gas phase, ligand-free synthesis; in particular we used two new generation cluster sources: the multiple ions cluster source (MICS)2 and the matrix assembly cluster source (MACS)3. The conventional magnetron-based cluster source is based on the sputtering of a single pure or alloy target under vacuum conditions with subsequent cluster aggregation via further collision with the aggregation gas. In the MICS the single magnetron is replaced with three independent magnetrons allowing the production of a wide range of nanoalloy clusters starting from pure targets. The great advantage of this source is the possibility to growth a wide range of samples via the controlled sputtering of pure targets, controlling both their structure (alloys, core@shell and shell@core) and composition by changing the mutual magnetron positions as well as their sputtering rate. For the present study we deposited binary Pt-Cu clusters with the same size and compositions, but different structures: alloy, core@shell and shell@core, in order to investigate the effect of the nanostructures on gas-phase catalytic and electro catalytic performance.

Audience Take Away:

- My work will be useful to the audience since I will present in detail the cluster creation in the field of catalysis, with the aim of reducing the Pt. The synthesis techniques I will present are new and with a huge number of advantages. My presentation will help their research in the catalysis field.

Biography

Dr Maria Chiara Spadaro got her PhD in Physics and Nanosciences at the University of Modena and Reggio Emilia at the beginning of 2016, working on NPs created with magnetron-based nanocluster source and characterizing them using TEM-related techniques. Her research experience is focused on the synthesis and study of nanoscale materials, including analysis of chemical and structural properties of nanostructures, surfaces and interfaces.

Her PhD work led to the award in electron microscopy applied to material science in 2016, from the Italian Society of Microscopic Science (SISM).

After postdoctoral appointments at the international center of electron microscopy (CIME) of EPFL, Lausanne, and at the University of Modena and Reggio Emilia, she moved to the Swansea University joining the Prof. Palmer's group, to work on the synthesis, with novel techniques, and characterization of binary NPs of interest in catalysis.

Bioconvection in Darcy-Forchheimer flow of Maxwell nanofluid using Cattaneo-Christov heat flux model

Muhammad Suleman
Faculty of Science, Jiangsu University, Department of Mathematics, Jiangsu University, China

Bioconvection has emerged as an important field of research due to its immense applications in environmental systems and engineering. In this article we investigated bioconvection in Darcy-Forchheimer flow of Maxwell nanofluid using Cattaneo-Christov model of heat flux under convective boundary conditions. The system of non-linear partial differential equations are converted into ordinary differential system through appropriate similarity transformations. The resulting system is solved by BVP4c. The impact of physical parameters are discussed through profiles of velocity, temperature, concentration, micro-organism volume fraction are discussed in detail.

Biography

My name is Dr. Muhammad Suleman. I did my PhD from Zhejiang University (ZJU), Hangzhou, China under the supervision of Prof. Dr. Wu Qingbiao. I am Assistant Professor in the Department of Mathematics, Comsats University Islamabad, Pakistan. Currently I am post doctoral research fellow in Jiangsu University, China. My research interests are Computational mathematics, fluid mechanics, fractional differential equations and analytical/numerical methods. I have published 15 SCI articles so far. I look forward to many more years of teaching and research.

Reaction pathways of methanol oxidation over a supported bimetallic catalyst

Luter Leke*, PhD., Ogbene Gilian Igbum, Ph.D.
Benue State University, Nigeria

The oxidation of methanol was studied over supported monometallic catalysts of copper and silver was studied over the supported bimetallics of the two metals over a range of temperature and contact times. This was done to ascertain the effect the bimetallics will have on the reaction pathways and subsequently on the product distribution of the oxidation products of this reaction owing to the enormous contributions the bimetallics have brought to the world of heterogeneous catalysis. Characterisation was performed by nitrogen adsorption and porosity measurements, XRD, and IR spectroscopy of adsorbed methanol and of adsorbed CO. These results indicated no crystalline phases of the loaded metals to be present. CO adsorption showed the presence of small cluster metal atoms on the surface of the catalysts. The reduction peaks from TPR studies also revealed the presence of partially oxidised and dispersed metal atoms. Infrared studies of methanol adsorbed on these sample catalysts revealed the presence of intermediate methoxy and formate species which have been reported to be formed in the course of the reactions. Silica as a support employed for its good thermal stability, fairly chemical inertness and surface areas as well as alumina, also a known for the aforementioned attributes and also its higher acidity were impregnated with the metal salts under investigation in both their mono and bimetallic forms. The bimetallic copper-silver interaction in the bimetallic was proposed to enhance the reduction of the silver that enhanced the selectivity to formaldehyde. Low conversions of methanol saw highest selectivities to formaldehyde. There was also a very pronounced effect of the supports on product distribution and activities with the alumina based samples being more active than the silica supported ones, with the product distributions on the alumina supported significantly showing high yields of DME while the silica showed high yield for methyl formate with COx and CH4 detected in very small quantities on all the catalysts within the parameters investigated.

Audience Take Away:

The various pathways of methanol oxidation as reflected in the reaction are outlined. The synergy of a bimetallic system in catalyst synthesis is also outlined. The essence of catalyst testing is outlined, by measuring the conversion, selectivity and yield of the various products. The importance of Characterisation of the synthesised materials is as well shown as it explains the behaviour of the catalysts synthesised under reaction conditions.

Biography

Luter Leke holds a BSc, Applied Chemistry of the University of Jos, an MSc, Industrial Chemistry of the prestigious University of Ibadan both in Nigeria and a PhD in Chemistry (Catalysis) of the University of Aberdeen, United Kingdom. He lectures chemistry at the Benue State University. Leke holds membership of several professional bodies which include; Institute of Chartered Chemists of Nigerian (ICCON), Chemical Society of Nigeria (C S N), Energy Institute, United Kingdom (E I), American Chemical Society (A C S) and Royal Society of Chemistry (R S C). He has published journal articles and also serves on the editorial board of some journals. He enjoys playing and watching soccer and tennis.

Investigation of Zr-promoted Cobalt based Fischer–Tropsch catalyst at high syngas conversion

Yahya Zamani*, Elham Yaghoobpour, Saeed Zarrinpashne, Akbar Zamaniyan, Ph.D.
Gas Research division, Research Institute of Petroleum Industry(RIPI), National Iranian Oil Company; West Blvd., Near Azadi Sports Complex
P.O.BOX 14665-137, Tehran, Iran

Fischer–Tropsch synthesis (FTS) is a route to produce liquid fuels from natural gas, coal and biomass. Ruthenium, iron and cobalt are most active metals for FTS. Cobalt preferentially produces more paraffinic hydrocarbons. Al2O3, TiO2 and SiO2 are currently used as supports for commercial cobalt catalysts. To facilitate the reduction of Co, which has strong interactions with Al2O3, researchers often add promoters such as Pd, Pt, Re, and Ru to the Cobalt catalysts. The cobalt based catalysts were prepared by a wet impregnation method. The catalysts were prepared in two steps: (step 1) Support of γ-alumina was stabilized by addition of Zr; (step 2) Co and Ru were deposited by wet impregnation to 25 nominal wt % and 0.2 wt % respectively. In Step 1, supports were impregnated with Zr using an aqueous Zircoium nitrate. The catalyst was dried at 120 oC then calcined at 400 ˚C for 3 h. For steps 2, Co and Ru were added to the Zr-stabilized support by wet impregnation method using Cobalt nitrate (Co(NO3)2.6H2O (merck, purity> 97%)) and Ru(NO)(NO3)3 (ACROS ORGANICS, in diluted nitric acid 0.01 ml/ml) targeting 25 wt % and 0.2 wt % of cobalt and Ru loadings for two steps. The final catalysts dried at 120 ˚C for 16 h and calcined at 400 ˚C for 3 h. The effect of zirconium promoter over Co-Ru/γ-Al2O3 was investigated. The Co loading was 25 wt. % on the catalysts. XRD, BET , TEM , and H2-TPR techniques were utilized to assess the catalysts phase, structure, morphology, and reduction temperature. Catalytic performance of the catalysts were studied in a fixed bed reactor. The catalysts were activated in situ with hydrogen at 400 ˚C for 16 h, then tested at the following conditions: T= 220 ˚C, P= 25 bar, H2/CO= 2, GHSV= 2nl.h-1.gCat-1. Both the promoter and the reaction conditions influence the product selectivity. The product distribution of hydrocarbons can be described by the Anderson-Schulz-Flory (ASF) equation: mn=(1-α) αn-1 with mn the mole fraction of a hydrocarbon with chain length n and the growth probability factor α independent of n. The Zr promoted catalyst exhibited a high catalytic activity and high selectivity to C5+ hydrocarbons in the FTS reaction.

Audience Take Away:

In this research, they will know about GTL catalyst including of catalyst preparation by impregnation method, catalysts characterization using different techniques (ASAP, H2-TPR,TEM.XRD,ICP), Test of the catalysts in the fixed-bed reactor effect of zr promoter on catalyst activity and products distribution.

- Other research institutes that have a reactor test system can use its results
- This catalyst is relatively suitable for use in the Fisher-Tropsch process.

Advantages of the catalyst:

- High conversion of carbon monoxide
- High hydrocarbon product
- High lifetime

Biography

I have graduated my BSC and MSc from Shahid Beheshty University in Tehran, Iran. I have completed my education as Ph.D in Organic chemistry in 2013 from Ferdowsi University of Mashhad in Iran. I was employed in RIPI about 17 years ago. I started my research on natural gas conversion field Contains: Syngas production process and catalysts, Fischer-Tropsch process and catalysts (Iron and Cobalt. I started my studies with laboratory tests on the activity and products selectivity on iron and cobalt catalysts, and continued my research with bench and pilot scales, which has worked for more than 1000 hours. I have published more than 100 papers and patents.I have paprticipated a lot of international conference as speaker including of 24th Coal conference in south Africa 2007,CFC 2011 in Japan ,CHISA 2010 and CHISA 2012 in Cheque republic, IGRC2014 in Denmark(poster) and IGRC2017 in Brasil.

CONTENTS

Synthesis of Co-Mn-Fe/γ-Al2O3 catalyst for light olefins production

Flor Shayegh*, Yahya Zamani, Mahsima Shamkhali
Research Institute of Petroleum Industry(RIPI), National Iranian Oil Company; West Blvd., Near Azadi Sports Complex P.O.BOX 14665-137, Tehran, Iran

In recent years, the researchers are interested in making light Olefins (C2-C4) from Syngas other than the methods of catalytic cracking of naphtha and dehydrogenation of alkanes. The catalysts of iron and cobalt mixed with Manganese used for conversion of Synthesis Gas to hydrocarbons have been extensively studied because of their characteristics such as selective formation of light Olefins in the C2-C4 range particularly Propene with a suppressed C1 product . Mn has been widely used as one of the promoters for unsupported Fe-based FT catalysts, particularly in promoting the production of C2-C4 Olefins. Some investigators have been working on operation parameters of Cobalt-based catalysts and showed that the Olefin contents of the product spectrum decreased with increasing pressure . In this work, Co-Mn-Fe/γ-Al2O3 catalyst was prepared a wet impregnation method. The catalyst was characterized using varying techniques such as XRD,H2-TPR, SEM and BET techniques. The effects of temperature, support, Mn to Co ratio on the catalytic performance of these catalysts have been investigated. It has been shown that [Mn]/[Co] molar ratio are important in controlling the catalytic activity . The catalyst gave the highest catalytic performance for the conversion of synthesis gas to light olefins.

Audience Take Away:

- In this research, the method of making catalyst by impregnation method, characteristics of the catalysts using different techniques (ASAP,H2-TPR,SEM.XRD), Test of the catalysts in the fixed-bed reactor ,Study of catalyst activity and products distribution.
- Other research institutes that have a reactor test system can use its results
- This catalyst is relatively suitable for olefin production.

Advantages :

  - High light olefin
  - High lifetime

Biography

I was born at1965 in Iran and completed my BSC and MSc in chemical engineering in 1989 from Sharif University of Technology in Tehran, Iran. And I completed my education as PhD in chemical engineering in 2010 from Sharif university of Technology .Title of PhD thesis is 'Optimizing structure of catalysts and development of kinetic parameters for synthesis gas to olefin reaction' .I have worked in Research Institute of Petroleum Industry from 1989.My major research on natural gas conversion field contains Syngas production process and catalyst, Fischer-Tropsch process and catalysts(Iron and Cobalt),Syngas to Olefins conversion ,process and catalysts preparation and kinetics. I have more than 70 papers (conference paper, ISI and internal papers) and some patents. I participated a lot of international conference as speaker including of 8th WCCE in Canada 2009, CHISA 2012,11NGCS in Noevay,IGRC2017 in Brasil.

Catalysis Events 2019

Catalysis and Chemical Science

March 11-13, 2019, Singapore
https://catalysiscongress.com/
Email: catalysis-2019@magnus-group.org

Catalysis and Green Chemistry

May 13-14, 2019, Tokyo, Japan
https://catalysis-conferences.com/
Email: greenchemistry@magnusmeetings.com

Catalysis, Chemical Engineering and Technology

September 16-18, 2019, London, UK
http://catalysisevents.com/
Email: catalysis@magnus-group.org

http://catalysisevents.com/