5th International Conference on

Green Chemistry and Technology

&

6th International Conference on

Environmental Chemistry and Engineering

July 24-26, 2017 Rome, Italy

Scientific Tracks & Abstracts

Day 1

Sessions

Day 1 July 24, 2017

Green Catalysis | Green Synthesis/Reactions | Green Chemistry

Session Chair
Shuji Akai
Osaka University, Japan

Session Co-Chair
Karine de Oliveira Vigier
University of Poitiers, France

Session Introduction

Title: Lipase-metal integrated catalysis for quantitative conversion of racemic alcohols into optically pure compounds

Shuji Akai, Osaka University, Japan

Title: Catalytic conversion of carbohydrates in the presence of choline chloride : Use of deep eutectic solvents

Karine de Oliveira Vigier, University of Poitiers, France

Title: Elucidation of the electronic structure of metal-oxo reactive species in porous media for the oxidation of methane and ethane

Konstantinos D. Vogiatzis, The University of Tennessee, USA

Title: Readily available homogeneous and heterogeneous catalysts for the cycloaddition of CO_2 to epoxides: A low carbon-footprint perspective

Valerio D' Elia, Vidyasirimedhi Institute of Science and Technology, Thailand

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Musa M. Musa, King Fahd University of Petroleum and Minerals, Saudi Arabia

Title: Flow microreactors enables green chemistry approach for organolithium chemistry

Aiichiro Nagaki, Kyoto University, Japan

Title: Expanding the reaction space of aldolases using hydroxypyruvate as a nucleophilic substrate

Virgil Helaine, Université Clermont Auvergne, France

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DOI: 10.21767/2471-9889-C1-002

Lipase-metal integrated catalysis for quantitative conversion of racemic alcohols into optically pure compounds

Shuji Akai
Osaka University, Japan

Hydrolase-catalyzed kinetic resolution (KR) of racemic alcohols in organic media is one of the most common approaches used to obtain optically pure alcohols and their corresponding esters. A wide range of hydrolases, such as lipases and esterases, have been utilized for KR, many of which are commercially available as solids immobilized on a support and exhibit high catalytic activity in various organic solvents. Unlike other enzymes, the hydrolases have advantages, such as robustness, high chemo- and stereo-differentiating ability, applicability to a wide range of non-natural substrates, and lack of cofactor dependency. In addition, the hydrolase-catalyzed KR of alcohols has distinct benefits in terms of mild reaction conditions as well as the ease and safety of operation and work-up. However, KR has an inherent limitation as it only gives a maximum 50% yield of products. In this symposium, we present a dynamic kinetic resolution (DKR) method to overcome this issue. DKR is performed using an integration of the lipase-catalyzed KR of racemic alcohols and the *in situ* racemization of the remaining less reactive enantiomers by V-MPS, in which the oxovanadium species is covalently bound to the inner surface of mesoporous silica (MPS) with a pore size of about 3–4 nm (Figure 1B). Its small pore size completely divides the racemization and kinetic resolution sites, and achieves the perfect compatibility between the oxovanadium moiety and lipases. By the combined use of these two catalysts, racemic alcohols were converted into the optically active esters (R)-3 with up to 99% isolated yield and 99% ee. The preparation of optically active cycloalkenes bearing all-carbon quaternary stereogenic centers was developed by direct use of the acyl moiety of the product. The practical application of these methods has been demonstrated by the asymmetric synthesis of bioactive natural products.

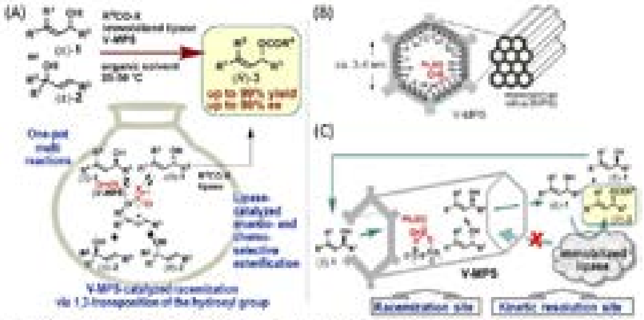

Figure 1. (A) Outline of the lipase/oxovanadium-integrated catalysis for dynamic kinetic resolution of racemic allyl alcohols. The absolute stereochemistry is shown as a representative example. (B) Structure of V-MPS. (C) The concept of reaction site separation for a dynamic kinetic resolution process using the narrow pores of MPS.

Biography

Shuji Akai obtained PhD degree in 1987 from Osaka University. After two years of Postdoctoral work as a JSPS Research Fellow at Osaka University, he was appointed as Assistant Professor at Osaka University and promoted to a Full Professor at University of Shizuoka in 2005. Since 2013, he has been a Full Professor at Osaka University. He was a Visiting Research Fellow with Professor Stephen L Buchwald at MIT during the year 1997–1998. He received the Inoue Research Award for Young Scientists (1987), the Pharmaceutical Society of Japan Award for Divisional Scientific Promotions (2003), and the Japanese Society for Process Chemistry Award for Excellence (2005 and 2011). His current research interests include Synthetic Organic Chemistry, Enzymatic Synthesis, Fluorine Chemistry, and Medicinal Chemistry.

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Notes:

Karine de Oliveira Vigier et al., Trends in Green chem, 3:2
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Catalytic conversion of carbohydrates in presence of choline chloride: Use of deep eutectic solvents

Karine de Oliveira Vigier and **François Jérôme**
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The catalytic conversion of carbohydrates to value added chemicals or platform molecules is the topic of numerous researches. One of the challenges is the use of a selective and stable catalyst, and also the nature of the solvent that allows the dissolution of highly concentrated carbohydrates which is environmental friendly. An interesting class of solvents is gaining more and more attention: Deep Eutectic Solvents (DES) or Low Melting Mixtures (LMM). Formation of these solvents can be obtained by simply mixing together two safe components, (cheap, renewable and biodegradable) which are capable of forming a eutectic mixture or a low melting mixture. One of the most widespread components used for the formation of these solvents is choline chloride (ChCl). ChCl is a very cheap, biodegradable and non toxic quaternary ammonium salts which can be either extracted from biomass or readily synthesized from fossil reserves (million metric tons) through a very high atom economy process. In combination with safe hydrogen bond donors such as carbohydrates, ChCl is capable of rapidly forming a DES/LMM. We have studied several catalytic conversions of carbohydrates. One of the reactions studied was the dehydration of fructose and glucose to produce 5-hydroxymethylfurfural. We have shown that high yield to HMF can be obtained when ChCl was added to the carbohydrates. Moreover, concentrated solution of carbohydrates could be used in some cases, which is a high advantage in the carbohydrates chemistry. Another reaction studied was the catalytic conversion of fructose to diformylfuran (DFF) in a one pot process. In all these studies, it was shown that ChCl can help control the selectivity of the reaction by providing interactions with the furanic derivatives avoiding their degradation. Some new insights of the mechanism will be provided.

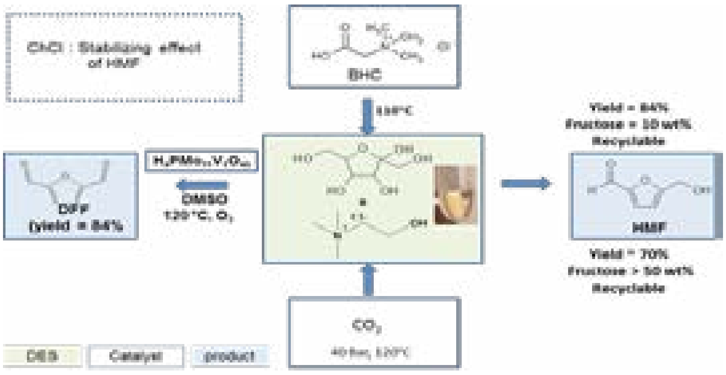

Figure 1: Use of choline chloride for the catalytic conversion of carbohydrates

Biography

Karine de Oliveira Vigier has her expertise in heterogeneous catalysis, deep eutectic solvents, ionic liquids, renewable carbon. Her main field of research consists of the development of unconventional media to assist the catalyst in the control of the selectivity for the conversion of biomass (carbohydrates, furanic derivatives, and glycerol) to fine chemicals and fuels. After a PhD in catalytic conversion of vegetable oils in France, she moved to Canada for a Postdoctoral position. She is now an Associate Professor at the Institute of Chemistry of Poitiers (IC2MP) in France since 2004. She has received the Young Researcher prize from the Catalysis Division of the French Chemical Society and she is the member of the Editorial Advisory Board of the *ACS Sustainable Chemistry & Engineering* journal.

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Konstantinos D Vogiatzis, Trends in Green chem, 3:2
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Elucidation of the electronic structure of metal-oxo reactive species in porous media for the oxidation of methane and ethane

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High-valent metal-oxo species attract considerable interest due to their catalytic role in oxygenation reactions as active intermediates. A synthetic route that has successfully applied in functional materials is the introduction of reactive species inside porous materials that mimic the nuclearity and reactivity of active sites of enzymatic analogues, such as the methane mono-oxygenase and non-heme enzymes. Metal-organic frameworks (MOFs) and zeolites are porous materials that can offer advantageous coordination environments for the formation of such highly reactive species. Two such examples will be discussed. The first is the iron-containing MOF, Fe0.1Mg1.9(dobdc) (dobdc4- = 2,5-dioxido-1,4-benzene-dicarboxylate), which was reported to catalyze the oxidation of ethane to ethanol in the presence of nitrous oxide. The catalytic activity of the iron-containing MOF was attributed to an uncommon high-spin iron (IV)-oxo intermediate. The second part of this talk is related to the unique $[Cu_3O_3]^{2-}$ ring intermediate deposited on the mordenite zeolite. The tricopper cluster site was reported to catalyze the oxidation of methane to methanol. The multireference character of this single-site active site affects its catalytic behavior and thus, its electronic structure was examined by multi-configurational wave function methods.

Biography

Konstantinos D Vogiatzis completed his BS in Chemistry at the University of Athens, Greece, in 2006 and he obtained his Master's (MSc) in Applied Molecular Spectroscopy from the University of Crete, Greece, in 2008. He received his PhD in 2012 from the Karlsruhe Institute of Technology, Germany, where he developed a highly accurate coupled-cluster scheme in the group of Prof. Wim Klopper. After an eight-month Post-doctoral appointment at the Institute of Nanotechnology at the Karlsruhe Institute of Technology, Germany, he moved to the University of Minnesota (UMN) in 2014 where he performed Post-doctoral Research in the group of Prof. Laura Gagliardi. His research at the UMN focused on the catalytic and sorption properties of metal-organic frameworks (MOFs), and on the development and application of strongly correlated methods. In 2016, he joined the University of Tennessee as an Assistant Professor of Theoretical and Computational Chemistry.

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Valerio D' Elia, Trends in Green chem, 3:2
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Readily available homogeneous and heterogeneous catalysts for the cycloaddition of CO_2 to epoxides: A low carbon-footprint perspective

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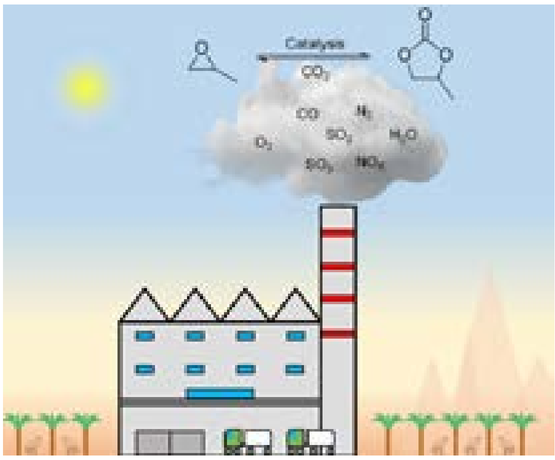
The conversion of CO_2 to chemicals is in the focus of academic and industrial research due to the high demand of viable strategies in alternative to the atmospheric release or geological segregation of carbon dioxide anthropogenic emissions. Cyclic organic carbonates represent a relevant class of chemicals that can be prepared from CO_2 by its cycloaddition to epoxides. Importantly they can be applied as chemical intermediates in the industry, as building blocks for polymers, as solvents and as additives in commercial products. Moreover, they are increasingly studied as useful chemical intermediates. A plethora of homogeneous and heterogeneous catalyst has been developed for the title reaction in the last decades, but, in spite of the exothermic nature of the cycloaddition process, only a small fraction of the published systems are able to promote this reaction under ambient conditions. Among such systems there are very simple halides of early transition metals used in combination with nucleophilic co-catalysts that take advantage of their high Lewis acidity for the step of ring opening of the epoxide substrate. Intriguing mechanistic aspects have been identified that suggest a bimetallic step of CO_2 activation when $NbCl_5$ is used as a catalyst. This effect has been observed as well for silica supported Nb atoms leading to an unprecedented cooperative effect for surface immobilized atoms in the activation of CO_2. We have recently shown that early transition metal halides of yttrium, scandium and zirconium can also convert CO_2 to cyclic organic carbonates when industrial waste flue gas was used as an impure source of CO_2, an observation that could pave the way for a direct and highly integrated conversion of CO_2 at the point of emission, thus circumventing the additional C-costs relative to purification, compression and transportation of CO_2. These systems will be reviewed along with other recently discovered, readily available catalysts for the title reaction.



Biography

Valerio D' Elia obtained his Master's in Chemistry from University of Perugia in 2001 and worked as a Scientist at Dompe Pharmaceuticals (L' Aquila, Italy). He joined the group of Oliver Reiser (Regensburg, Germany) for his Doctoral Studies in 2005. After a period (2009-2010) at the Ludwig Maximilian University in Munich under Hendrik Zipse, he joined Jean Marie Basset at King Abdullah University of Science and Technology (KAUST) Catalysis Center (Saudi Arabia). Since August 2015, he has been a Faculty Member in the School of Molecular Science and Engineering at the Vidyasirimedhi Institute of Science and Technology (VISTEC) in Rayong, Thailand. His main research interests are CO_2 Chemistry and Catalysis.

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Musa M Musa et al., Trends in Green chem, 3:2
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A single enzymatic approach for deracemization of secondary alcohols

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Controlling enantioselectivity of alcohol dehydrogenase-catalyzed transformations using site-directed mutagenesis enabled their used in racemization of enantiopure secondary alcohols and in deracemization of racemic secondary alcohols. Controlled racemization of enantiopure secondary alcohols is achieved using various mutants of secondary alcohol dehydrogenase from *Thermoanaerobacter ethanolicus* (TeSADH) and in the presence of the reduced and oxidized forms of its cofactor nicotinamide-adenine dinucleotide. We also developed a deracemization method for secondary alcohols that uses a single mutant of TeSADH in two steps. A single mutant of TeSADH enables the non-stereoselective oxidation of racemic alcohols to ketones, followed by a stereoselective reduction reaction for the resulted ketone. The key component in this deracemization approach is the ability to control the TeSADH-catalyzed transformations using protein engineering and medium engineering. Varying the amounts of acetone and 2-propanol co-substrates controls the stereoselectivities of the consecutive oxidation and reduction reactions, respectively. We used one enzyme to accomplish deracemization of secondary alcohols with up to >99% ee and >99% recovery in one pot and without the need to isolate the prochiral ketone intermediate. This deracemization approach is simple, efficient and environmentally benign.

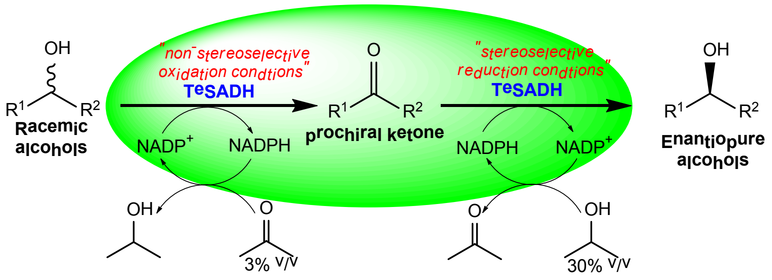

Figure 1: Single enzymatic approach for secondary alcohols using *Thermoanaerobacter ethanolicus* secondary alcohol dehydrogenase.

Biography

Musa M Musa received his PhD from the University of Georgia under the supervision of Prof. Robert S Phillips working in biotransformation in non-aqueous media. He then carried research with Prof. Mark D Distefano as a Postdoctoral Associate at University of Minnesota, where he focused on synthesis and evaluation of protein farnesyltransferase inhibitors and protein labeling. In 2009, he joined King Fahd University of Petroleum and Minerals (KFUPM) as Assistant Professor. He is currently an Associate Professor of Chemistry at KFUPM. His research interests include employing enzymes in organic synthesis. More specifically, he is interested in enzyme-catalyzed racemization, deracemization, and dynamic kinetic resolution of alcohols.

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Notes:

Aiichiro Nagaki, Trends in Green chem, 3:2
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Flow microreactors enables green chemistry approach for organolithium chemistry

Aiichiro Nagaki
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Protecting-group-free synthesis has received significant recent research interest in the context of ideal synthesis and green sustainable chemistry. In general, organolithium species react with electrophilic functional groups very rapidly, and therefore such functional groups should be protected before an organolithium reaction, if they are not involved in the desired transformation. If organolithium chemistry could be free from such a limitation, its power would be greatly enhanced. A flow microreactor enables such protecting-group-free organolithium reactions by choosing the appropriate residence time and the reaction temperature. Organolithium species bearing alkoxycarbonyl, nitro, and ketone carbonyl groups can be generated and reacted with various electrophiles using a flow-microreactor system. In addition, asymmetric carbolithiation of conjugate enynes can be also achieved without the epimerization of a configurationally unstable chiral organolithium intermediate based on precise control of the residence time using a flow microreactor. In this presentation, we report that a flow microreactor system enables the generation of various unstable organolithium compounds.

Biography

Aiichiro Nagaki received his PhD in 2005 from Kyoto University under the supervision of Professor Jun-ichi Yoshida. He worked with Professor Hiroaki Suga, Tokyo University from 2005 as a Postdoctoral Fellow. In 2006, he became an Assistant Professor at Kyoto University. He was promoted to Junior Associate Professor in 2013. His current research interests are Organic Synthesis, Polymer Synthesis, and Microreactor Synthesis. He has received several awards which includes Takeda Pharmaceutical Co., Ltd. award in Synthetic Organic Chemistry, Japan (2012), Incentive Award in Synthetic Organic Chemistry, Japan (2012), and Young Innovator Award on Chemistry and Micro-Nano Systems (2013).

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Virgil Helaine et al., Trends in Green chem, 3:2
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Expanding the reaction space of aldolases using hydroxypyruvate as a nucleophilic substrate

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[2]National Center for Scientific Research (CNRS), France
[3]Sigma Clermont, France
[4]Institut de Chimie de Clermont-Ferrand, France

Aldolases are key biocatalysts for stereoselective C–C bond formation allowing access to polyoxygenated chiral units through direct, efficient, and sustainable synthetic processes. The aldol reaction involving unprotected hydroxypyruvate and an aldehyde offers access to valuable polyhydroxy-α-ketoacids. However, this undescribed aldolisation is highly challenging, especially regarding stereoselectivity. This reaction was explored using biocatalysts, a collection of aldolases selected from biodiversity. Several enzymes were found to produce the desired hexulosonic acids from hydroxypyruvate and D-glyceraldehyde with complementary stereo-selectivities. One of them was selected for the proof of concept as a biocatalytic tool to prepare five (3S, 4S) aldol adducts through an eco-friendly process.

Biography

Virgil Helaine has completed his PhD from Clermont-Ferrand University, France. He has left for Darmstadt (Germany) where he has joined Prof. W D Fessner's group. Since 2000, he is an Assistant Professor in the Institute for Chemistry of Clermont-Ferrand (France) and his field of interest is focused on biocatalysis especially the development of tools for eco-compatible synthesis: discovery and study of new enzymes, and their orchestration in multienzymatic cascade processes towards compounds of biological interests.

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Notes:

Day 1 July 24, 2017

Environmental Chemistry | Environmental Toxicology and Mutagenicity | Renewable Energy Sources and Storages

Session Chair	Session Co-Chair
Angelo Nacci	**Maria Michela Dell'Anna**
University of Bari, Italy	Polythecnic University of Bari, Italy

Session Introduction

Title: An assessment of air quality in the surrounding holy places of Mecca, Saudi Arabia during Hajj
Haider A Khwaja, University at Albany, USA

Title: Nanostructured materials for green catalysis
Angelo Nacci, University of Bari, Italy

Title: Carbon-enhanced manufacturing and digitalization supporting cycle economy
Dominik Rohrmus, Siemens AG, Germany

Title: Catalytic activity and recyclability of polymer supported palladium or nickel nanoparticles in organic reactions in water
Maria Michela Dell'Anna, Polythecnic University of Bari, Italy

Title: A novel mechanism for BPA-triggered hepatic steatosis
Sijun Dong, Institute of Urban Environment - CAS, China

Title: Electrocatalytic production of hydrogen using iron sulfur cluster
Khalaf M Alenezi, University of Hail, KSA

Title: Heavy metals in seawater from Marmara sea, Istanbul
Gökberk Kara, Marmara University, Turkey

Title: Dosing of proper oxidizing agents pretreatment to Kalatuwawa water to reduce the Trihalomethane (THM) formation in drinking water
Jayalal L P R Wijesinghe, National Water Supply and Drainage Board, Sri Lanka

Title: Preparation of Yb^{3+} doped microspherical BiOI and its photocatalytic activity for the degradation of rhodamine B in water
Linping Zhang, Donghua University, China

Title: Concentration, temperature and kinetics studies of *Kola nitida* leaves extract in corrosion prevention
Adebayo Oluwafemi Lawrence, College of Education Ikere, Nigeria

Title: Assessment of Polynuclear Aromatic Hydrocarbons (PAHs) in local steak (suya) samples in Makurdi town, Benue State-Nigeria
Ubwa S T, Benue State University, Nigeria

Title: Using electrocoagulation to remove chloride and ammonium from reject brine treated by solvay process
Miada A Ali, United Arab Emirates University, UAE

Haider A Khwaja et al., Trends in Green chem, 3:2
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An assessment of air quality in the surrounding holy places of Mecca, Saudi Arabia during Hajj

Haider A Khwaja[1], **Omar S Abu-Rizaiza**[2], **Azhar Siddique**[3], **Jahan Zeb**[2] and **Donald R Blake**[4]
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[2]King Abdulaziz University, Saudi Arabia
[3]Qatar Environment & Energy Institute, Qatar
[4]University of California, USA

The associations of exposure to air pollution and adverse human health effects have been demonstrated in many epidemiologic studies. Hajj, an annual pilgrimage of Islam, draws millions of pilgrims from more than 200 countries for religious rituals in Mecca, Saudi Arabia. The city is surrounded by mountains with a population of 1.7 million, which gets doubles or even more during Hajj. The city centers on the Grand Mosque (Masjid Al-haram), connected with the network of tunnels. Main Hajj pilgrimage route for five days extends 20 km to the east and includes *"Mina"*, *"Arafat"* and *"Muzdalifah"*. A detailed study was conducted in Mecca, its tunnels, and surrounding holy places during Hajj (October 13-17, 2013). Spatial and temporal variations in total suspended particulate (TSP), PM10 , PM7 , PM2.5 , PM1 , ozone (O3), and black carbon (BC) levels along the route were recorded using portable monitors and GPS to assess the status of air quality. This is the first study to elucidate the exposure to air pollutants among pilgrims. Extremely high levels of all pollutants were observed during the intensive measuring periods. For example, the PM7, PM2.5, O3, and BC concentrations of up to 9,433 µg/m3, 484 µg/m3, 444 ppb, and 468 µg/m3, respectively, were observed. Results of this investigation revealed that most routes had on average exceeded the World Health Organization (WHO) standards for PM10 and PM2.5. The reasons for the high air pollutants concentrations are most probably high volume of traffic, construction work, re-suspension of particles, and geographical conditions (arid regions). The pilgrim's longer trip duration lead to their highest whole trip exposure to air pollutants, which indicate that they are possibly subject to higher health risk. Better understanding of air pollution exposure and their determinants in the environments will contribute to the development of more appropriate exposure reductive strategies and have significant public health meanings.

Biography

Haider A Khwaja has 27 years of solid research experience on environmental projects. He is the Director of the Laboratory of Inorganic Chemistry at the Wadsworth Center, NYSDOH. He is a Faculty Member at the Department of Environmental Health Sciences, School of Public Health, University at Albany, where he teaches and mentors graduate and undergraduate students. He has been carrying out various environmental projects in USA and in developing countries. Active research programs include: 1. Effects of particulate matter on daily morbidity and mortality due to cardiovascular and pulmonary diseases in urban areas; 2. Chemical characteristics of fine particles responsible for the observed health effects; 3. Exposure and health impacts related to outdoor and indoor air pollution including studies of volatile organic compounds (VOCs), polycyclic aromatic hydrocarbons (PAHs), diesel vehicle emission, air toxins, and indoor allergens; 4. Water and human health issues such as drinking water quality and human health risks associated with water contaminants.

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Notes:

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Nanostructured materials for green catalysis

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Transition-metal Nanoparticles (NPs) are attracting a great deal of attention in almost any scientific and technological field, including catalysis, where nanoscale materials are becoming more prevalent in a wide range of applications such as fuel conversion, pollution abatement and fine chemical production. Nowadays, many researchers are exploiting the high activity and selectivity of nanocatalysts to develop greener and waste-minimized processes. During the last decade, we exploited nanostructured catalysts based on several metals like Pd, Cu, Au, Zn and Ti to perform a wide range of organometallic reactions (Heck, Suzuki, Ullmann, Stille, carbonylations, cyclopropanations, C-H activations, hydrodehalogenations and CO_2 photoreduction) under environmentally friendly conditions given by the absence of phosphane ligands and using neoteric solvents (ionic liquids, water, emulsion mixtures and so on) as green reaction media. This lecture deals with our recent advances in controlling the catalyst performances by choosing properly the nature of both the ionic liquid and the nanocatalyst.

Biography

Angelo Nacci completed his PhD in Chemical Sciences in 1994 at Bari University (Italy). He was a Researcher in Organic Chemistry at the Chemistry Department of Bari University. In 2001, he was a Visiting Researcher at TUM University of Munich (Germany) and in 2005 he became an Associate Professor of Organic Chemistry. He is currently the President of Chemistry Courses Degree at Bari University. His research interests are focused on: organometallic chemistry in ionic liquids; green nanocatalysis; CO_2 capture and valorization and synthesis and recycling of bioplastics. He is the co-author of almost 70 publications in major journals and has one patent.

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Dominik Rohrmus, Trends in Green chem, 3:2
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Carbon-enhanced manufacturing and digitalization supporting cycle economy

Dominik Rohrmus
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The global challenge climate change calls for answers beyond the pure optimization of resources and energy consumption in manufacturing - a major CO_2 causer. CO_2 as a supply for new synthetic raw materials and products as well as markets is a new long-term approach to establish a green cycle economy. We define green cycles as CO_2 sinks. The Siemens green cycle vision for green production and green raw materials as displayed in Figure 1 opens new manufacturing models and new product markets to provide an answer for the world's hunger for materials. These materials have a promising future for non-food related components such as electronic parts. Green cycle factories apply the concept of green cycles to the discrete manufacturing industries. The prerequisites are renewable energy and chemistry production technologies, which are synthesizing fuels and materials for manufacturing from CO_2 sources. The world has to focus on renewable supplies, which fulfill the demands of future manufacturing technologies in terms of additive manufacturing processes that are then mainly using carbon materials. Our new findings can help to contribute to a greener future as carbon-based materials come from renewable, biodegradable resources. The transformation process requires new competitive manufacturing systems in a decentralized and digitalized manner. An additive manufacturing process based on this carbon feedstock is one promising application field with the advantage to transfer the carbon load into discrete products. Hence, low carbon in the atmosphere can be realized by green cycles and advanced carbon-based materials and manufacturing.

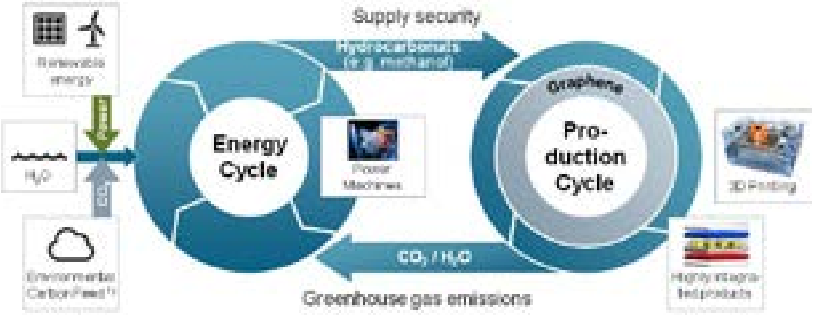

Figure 1: Vision of future energy and production cycles economy

Biography

Dominik Rohrmus works at Siemens Corporate Technology in Munich, Germany in different functions in the area of manufacturing development and production equipment realization since 2005. In 2009, he founded the company program, Sustainable Production Engineering and rolled several demonstrator projects company-wide out. In particular energy efficient production planning and technology on the shop-floor set the focus of that program. Also cycle economy and cycle business development in cooperation with Siemens business units and external partners is part of the program and yield already several pilot projects. Since 2013, he is the Head of the research group, Manufacturing Systems Engineering at Siemens Corporate Technology. The research group is responsible for shop-floor equipment standardization and development of the future for the Siemens factories worldwide.

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Notes:

Maria Michela Dell'Anna et al., Trends in Green chem, 3:2
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Catalytic activity and recyclability of polymer supported palladium or nickel nanoparticles in organic reactions in water

Maria Michela Dell'Anna[1], **Matilda Mali**[1], **Giuseppe Romanazzi**[1], **Antonino Rizzuti**[1], **Cristina Leonelli**[2] and **Piero Mastrorilli**[1]
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An insoluble palladium catalyst (*Pd-pol*) was obtained by copolymerization of the metal containing monomer Pd(AAEMA)2 [AAEMA− = deprotonated form of 2-(acetoacetoxy)ethyl methacrylate] with ethyl methacrylate (co-monomer) and ethylene glycol dimethacrylate (cross-linker), followed by *in situ* reduction of Pd(II) to Pd(0), to give polymer stabilized metal nanoparticles. The good swellability in water exhibited by *Pd-pol* rendered it an ideal potential catalyst for reactions carried out in a green solvent, such as water, since the migration of the reagents to the active sites would not be hampered by the solid support. With the aim to develop innovative catalytic processes that enable chemical transformations to be performed under mild and sustainable conditions with high efficiency, we decided to evaluate the catalytic activity of *Pd-pol* for several important organic reactions using water as solvent. *Pd-pol* resulted highly active and selective in catalyzing (figure 1): the Suzuki-Miyaura coupling between aryl bromides or activated aryl chlorides and phenylboronic acid; the oxidation of benzyl alcohols to aldehydes; the reduction of quinolines and nitroarenes by H_2 or $NaBH_4$. *Pd-pol* was recyclable for several consecutive runs (for example, at least 12 times in the nitroarene reduction). TEM analyses carried out on the catalyst showed that the active species were supported palladium nanoparticles having a mean size of 4 nm, which did not aggregate with the recycles. Recently, due to their low cost, Ni catalysts have been employed in several organic reactions (mainly hydrogenations). In this context, we synthetized a Ni catalyst similar to *Pd-pol*, starting from $Ni(AAEMA)_2$ and we employed it as active and recyclable, insoluble catalyst for the reduction of different nitroarenes to give the corresponding anilines, under sustainable conditions. All these results proved that the proposed Pd or Ni based composite materials are excellent hybrid structures as efficient and reusable catalysts.

Biography

Maria Michela Dell'Anna completed her PhD in "Chemistry of materials for special uses" at University of Reggio Calabria (Italy), giving a dissertation on "Synthesis and characterization of new transition metal complexes: Aerobic oxidation of organic substrates and C-C bond forming reactions". During her PhD studies, she joined for one year the research group of Prof. M Cowie in the Chemistry Department of University of Alberta (Canada), where she worked on the synthesis and characterization of bimetallic complexes. Since 2000, she has been Assistant Professor in Chemistry at Polytechnic of Bari. Since 2012 she has been the Editor of the journal *Recyclable Catalysis*, merged with the journal *Catalysis for Sustainable Energy*. Her research interests are focused on: i) polymer supported metal catalysts; ii) green nanocatalysis; iii) platinum complexes and iv) risk assessment. She is co-author of almost 45 publications in major journals and more than 20 communications in congresses.

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Notes:

Sijun Dong, Trends in Green chem, 3:2
DOI: 10.21767/2471-9889-C1-002

A novel mechanism for BPA-triggered hepatic steatosis

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Exposure to Bisphenol A (BPA) has been linked to the increased incidence of Non-Alcoholic Fatty Liver Disease (NAFLD): The hepatic manifestation of metabolic syndrome. However, the related underlying mechanisms remain unknown. Given that microRNAs (miRNAs) are widely recognized as the key regulators of lipid metabolism and the potential mediators of environmental effects, this study aimed to examine whether exposure to BPA triggered hepatic lipid accumulation and to further determine if adverse effects of BPA may be modulated in part through miRNAs. Male post-weaning C57BL/6 mice were exposed to 50 μg/kg/day BPA or corn oil for 90 days by oral gavage. We found that insulin resistance, and impaired hepatic lipid accumulation and increased serum triglycerides (TG) existed concomitantly in the BPA exposed mice. In addition, BPA exposure caused significant reduction in miR-192 expression in both mice liver tissues and human HepG2 cells, which were accompanied by significant up-regulation of SREBF1 (a key transcription factors that is capable of activate lipid synthesis) and subsequent expression of lipogenic genes. Bioinformatic and *in vitro* studies suggested that miR-192 acted to the 3'UTR of SREBF1 directly, resulting in profound dysregulation in hepatic lipid homeostasis. Inhibition of miR-192 led to higher TG levels and increased hepatic lipid accumulation by enhancing SREBF1 processing. In contrast, the opposite results were observed with overexpression of miR-192, which downregulated SREBF1 expression. Most importantly, we also showed that *in vivo* and *in vitro* overexpression of miR-192 effectively prevented BPA induced hepatic lipid accumulation, which was independently of insulin resistance. In conclusion, this study showed a novel mechanism that exposure to BPA may up-regulate SREBF1 through inhibition of miR-192 in the liver, thereby contributing to NAFLD.

Biography

Sijun Dong has completed his PhD in 2004 in Biochemistry and Biotechnology, Tokyo University of Agriculture and Technology, Japan. He is the Professor of Environmental Sciences, Chinese Academy of Sciences. He has published more than 50 papers in reputed journals. His research interest is about Environmental Molecular Toxicology and Chinese Medicines and Environmental Health.

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Notes:

Khalaf M Alenezi, Trends in Green chem, 3:2
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Electrocatalytic production of hydrogen using iron sulfur cluster

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In response to the energy crisis, rising fossil fuel costs and global climate warming, this study focuses on the electrocatalytic reduction of proton into hydrogen using an iron sulfur cluster in the presence of pentafluorothiophenol. The direct reduction of pentafluorothiophenol at vitreous carbon electrode occurs at Ep -1.3 V vs. Ag/AgCl in $[Bu_4N][BF_4]$-DMF solution. Interestingly, in the presence of $[Fe_4S_4(SPh)_4][Bu_4N]_2$, the reduction potential shifts significantly to -0.98 V vs. Ag/AgCl. Based on gas chromatography analysis, the formation of H2 has been confirmed with a current efficiency of catalyst. 63% after two hours, while the chemical yield at the carbon electrode was about 46%. On the other hand, no H2 gas was detected without catalyst. Importantly, the increment of the concentration of acid (up to 18 equivalents) led to a positive shifting in the reduction potential until a value of 0.18 V. These results reflect the exquisite electrocatalytic efficiency of the protein-like iron sulfur cluster in Hydrogen Evolution Reaction (HER).

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Notes:

Gokberk Kara et al., Trends in Green chem, 3:2
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Heavy metals in seawater from Marmara sea, Istanbul

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In Istanbul, where dense industrialization and dense population are located, people can use Marmara Sea for recreational reasons. The beaches in which they interacted with the sea were selected primarily for the determination of heavy metal pollution. This study proposed to investigate the quality of seawater to protect health of people which do recreational activities such as swimming. Cr, and Zn concentrations and pH, temperature in seawater samples taken weekly from Kucuksu, Fenerbahce and Suadiye beaches in Asian side of Istanbul were investigated between 9 February 2009 and 4 May 2009. Measured temperature values varied from 7.1 to 27.6^{0}C and measured pH values varied from 8.15 to 8.47. The Cr and Zn concentrations analyzed by the Inductively Coupled Plasma Mass Spectrometry (ICP-MS) were under the limit values by the Turkish Water Pollution Control Regulation published by the Ministry of Environment and Urbanization. These findings indicate that there is no significant threat to aquatic life and human health from these heavy metals in sea water in Marmara Sea.

Biography

Gokberk Kara has completed his under-graduation in the Environmental Engineering Department of Sakarya University in 2007. He is a Master's degree student in Environmental Engineering Department of Marmara University and is also working at the RSK Environmental Consultancy Service in Istanbul, Turkey.

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Notes:

Jayalal L P R Wijesinghe et al., Trends in Green chem, 3:2
DOI: 10.21767/2471-9889-C1-002

Dosing of proper oxidizing agents pretreatment to Kalatuwawa water to reduce the Trihalomethane (THM) formation in drinking water

Jayalal L P R Wijesinghe, Nishantha D P Welikala, K P R S Samarasinghe and **Ranjith C Perera**
National Water Supply and Drainage Board, Sri Lanka

Kalatuwawa water treatment plant consists of aeration, coagulation, flocculation, sedimentation, filtration and disinfection. Existing aeration is not enough to oxidize the inorganic and organic impurities in Kalatuwawa raw water, therefore prechlorine is used as oxidizing agent in Kalatuwawa. Analytical results revealed that during the years 2000–2012, the Kalatuwawa raw water contained high concentration of ammonia (0.578±0.469 mg/dm^3), and highest concentration of ammonia 1.92 mg/dm3 was reported at the bottom of the reservoir, high concentration of iron (0.751±0.643 mg/dm^3), and the highest concentration of iron 12 mg/dm^3 was reported at the bottom of the reservoir. The color levels were 11.571±7.271 Hz and the highest level of color, 90 Hz was reported at the bottom of the reservoir. Pre chlorination where chlorine is utilized not only oxidize the iron, manganese, ammonia and organic compounds but also reacts with naturally occurring organic matter present in water to produce a group of organic compounds as a byproduct arising from chlorination which was classified as Trihalomethane (THM). THMs are often used as indicator compounds for other DBPs. The four main THM compounds found in abundance are chloroform ($CHCl_3$), bromodichloromethane ($CHCl_2Br$), dibromochloromethane ($CHClBr_2$) and bromoform ($CHBr_3$). Many factors which will affect the THM formation are concentration and type of precursors, type of disinfectant and concentration and the dosing point, temperature, pH, contact time and the length of the distribution network. This study is basically investigating THM formation without prechlorination where potassium permanganate ($KMnO_4$) is used as pretreatment to remove the organic and inorganic impurities. Laboratory analysis was carried out using Jar test apparatus with potassium permanganate to remove the impurities. Analytical results revealed that 90% of iron was removed with 0.3-0.6 mgdm-3 dosage of potassium permanganate and the same time manganese level is within SLS 614: 2013. THM levels were monitored using GC–ECD couple to purge and trap system where the THM levels were reduced significantly (67%).

Biography

Jayalal L P R Wijesinghe graduated from University of Colombo, Sri Lanka with a BSc (Hons) degree. After graduation, he has joined the Department of Chemistry, University of Colombo as a Demonstrator then as a Researcher. He has obtained PG Diploma in the field of Toxicology and MSc degree in the field of Analytical Chemistry from the same university. He has started his water sector career as a Regional Chemist attached to the National Water Supply & Drainage Board in North Central Province of Sri Lanka. After successful completion of eight years of regional works, he was promoted to the Senior Chemist position in NWSDB. Presently he is working as a Chief Chemist in NWS&DB in Sri Lanka. He has gained 22 years of experience in the field of Water Quality Monitoring with the operation of high end analytical instruments – AAS with GTA, GC/MS, etc. He has published twelve research papers in local and international journals. He has undergone many training programs locally as well as internationally like – Lake Water Quality Management course in Japan, LC/MS training course at Waters in India, Analytical Skills Development Course in Helsinky University in Finland, etc. He is a Fellow Member of the Institute of Chemistry, Ceylon and also a Chartered Chemist.

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Notes:

5th International Conference on
Green Chemistry and Technology
&
6th International Conference on
Environmental Chemistry and Engineering
July 24-26, 2017 Rome, Italy

Linping Zhang et al., Trends in Green chem, 3:2
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Preparation of Yb^{3+} doped microspherical BiOI and its photocatalytic activity for the degradation of Rhodamine B in water

Linping Zhang, Zengqiang Ma and **Ruyi Xie**
Donghua University, China

Bismuth oxychloride (BiOI) has a good visible light responsive property due to their relatively narrow band gap, and its photocatalytic performance is further improved by doping ytterbium ions (Yb^{3+}) which could be attributed to stronger optical absorption in UV-visible light region, effective separation of the photogenerated electron-hole pairs, and the capacity of Yb^{3+} ions to up-convert near-IR light into visible-light and UV light. In this study, a facile solvothermal method was adopted to synthesize different Yb^{3+} ions doped BiOI photocatalysts. The doped photocatalysts with molar ratios of 0, 0.5, 1, 1.5, 2 and 2.5% Yb^{3+} ions were prepared and 2% Yb^{3+} ions doped BiOI exhibited the highest photocatalytic degradation efficiency, which was 2 times higher than that of pure BiOI. As-prepared photocatalysts were further studied through SEM, XRD, UV–Vis DRS and free radical capture experiments, etc. which indicated that the doping ions entered into Lattice of BiOI photocatalysts and improved the photocatalytic performance. This work provided some potential application of Yb^{3+} doped BiOI for the degradation of organic contaminants in water.

Biography

Linping Zhang has completed her PhD from the Chinese University of Hong Kong. She is an Associate Professor of Donghua University in China. She has published more than 45 papers in reputed journals.

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Notes:

5th International Conference on

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&

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July 24-26, 2017 Rome, Italy

Workshop

Day 2

Marcelo E Domine, Trends in Green chem, 3:2
DOI: 10.21767/2471-9889-C1-002

Marcelo E Domine

Instituto de Tecnología Química, (UPV – CSIC), Spain

Sustainable processing of biomass and its derivatives

Lignocellulosic biomass from agricultural and forest residues ¾which does not compete with land use for other crops or for food production¾ is presented as an alternative for fuels and/or chemicals production, thus reducing our fossil fuels dependence. Nowadays, the processes of transformation of renewable raw materials (i.e. vegetal biomass) for the production of hydrocarbons and other chemical products are, in general, more expensive than the conventional processes, making the valorization processes for the biomass and the obtained bio-products not competitive with their analogues derived from petroleum. For this reason, a major challenge for chemists is to try to develop new (chemo-, bio-, combined systems) catalytic routes to convert biomass and its derivatives into fuels and chemicals through sustainable and economically viable processes in bio-refineries.

In this context, and aligned with the new bio-economy and zero-waste concepts, the new bio-refineries should produce these bio-products for fuels and chemicals applications by reducing wastes, this including both decreasing of side-products formation and residual effluents valorization in an integrated approach.

The workshop will be addressed to scientists, experts and students participating in the congress from both industry and academia whose are active in the area of biomass valorization via thermo-chemical and biological processes. Emphasis will be placed on the utilization of lignocellulosic biomass (including non-edible crops or low quality oils), which do not compete with food. In terms of conversion processes, the use of green catalytic methodologies (mainly heterogeneous catalysis) will be discussed. Moreover, alternative biomass-based products that are safer and have a reduced environmental footprint will be discussed, along with the integrated bio-refinery and energy conservation concepts. The issue of "metrics" in assessing the economic and environmental impact of biomass conversion to various products will also be considered.

Biography

Marcelo E. Domine completed his PhD at the Polytechnic University of Valencia (Spain) in 2003 under the guidance of Prof. A. Corma, and postdoctoral studies at the IRCELYON - CNRS (France, 2005-07). In 2008, he re-joined the Instituto de Tecnología Química (UPV-CSIC) of Valencia, Spain as Scientific Researcher of CSIC. His current research involves the synthesis and characterization of solid catalysts and their application in sustainable chemical processes, mainly focusing on new biomass-derivatives transformations and wastes valorization into fuels and valuable chemicals. He is co-author of more than 55 publications (also including several patent applications). He has presented over 18 invited conferences around the world. He has acted as Guest Managing Editor of Catalysis Today, and also as Reviewer in many renowned scientific journals in catalysis and fuels areas. He is actually the representative of CSIC (Spain) at the EERA Program – JP-Bioenergy (European Commission).

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5th International Conference on

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July 24-26, 2017 Rome, Italy

Scientific Tracks & Abstracts

Day 2

Green Materials | Green Energy | Green Chemistry

Session Chair
Vassiliki-Alexandra Glezakou
Pacific Northwest National Laboratory, USA

Session Co-Chair
Takeo Sasaki
Tokyo University of Science, Japan

Session Introduction

Title: Molecular simulations turn 'green': An integrated approach to accelerate the development of CO_2 capture solvents

Vassiliki-Alexandra Glezakou, Pacific Northwest National Laboratory, USA

Title: Photo-detachable adhesives composed of photo-depolymerizable Poly(olefin sulfone)s

Takeo Sasaki, Tokyo University of Science, Japan

Title: Vanillin: A renewable and versatile platform chemical for sustainable polymers

Joseph F. Stanzione III, Rowan University, USA

Title: Hydrogen peroxide - oxidation reactions under microwave irradiation

Dariusz Bogdal, Cracow University of Technology, Poland

Title: Supercritical fluid technology for greener processes

Youn-Woo Lee, Seoul National University, Korea

Title: Graphene-based material for oil spill removal

Annalisa Pola, Eni S.p.A, Italy

Title: Chemical markers for the characterization of bioaerosol

Francesca Buiarelli, University of Rome "La Sapienza", Italy

Title: Clean and sustainable liquid hydrogen storage materials

Chang Won Yoon, Korea Institute of Science and Technology, Republic of Korea

Title: Challenges of green chemistry for value added products

Ahindra Nag, Indian Institute of Technology, India

Title: Waste biomass derived aqueous extracts as alternative green solvent media for organic transformations

Diganta Sarma, Dibrugarh University, India

Title: Water quality of the Chelif river in the Mostaganem area (North-West of Algeria)

Batoul Benkaddour, Mostaganem University, Algeria

Title: Global atmospheric emissions of toxic heavy metals from anthropogenic sources under multi-scale regions

Hezhong Tian, Beijing Normal University, China

Title: Removal of oil hydrocarbons using the grass *Panicum máximum* and a bacterial consortium in contaminated soil

S M Contreras-Ramos, CIATEJ, Mexico

Title: Physicochemical and bacteriological analyses of water samples from hand dug wells in Lafia Metropolis

Abel Augustine, Federal University Lafia, Nigeria

Title: COX free Hydrogen production for fuel cell applications using cobalt incorporated carbon supported material

Aytak Mammadli, Gazi University, Turkey

Title: Development of a simple biogas digester as a source of renewable energy and sustainable livelihood

Lamfu Fabrice Yengong, University of Buea, Cameroon

Title: Determination of residues levels of seven pesticides in tomatoes samples taken from three markets in Khartoum state

Ahmed Hammad, University of Khartoum, Sudan

Vassiliki-Alexandra Glezakou, Trends in Green chem, 3:2
DOI: 10.21767/2471-9889-C1-002

Molecular simulations turn ‘green’: An integrated approach to accelerate the development of CO_2 capture solvents

Vassiliki-Alexandra Glezakou
Pacific Northwest National Laboratory, USA

The ever-increasing carbon footprint from post-combustion large point sources has made greenhouse emissions one of the most urgent environmental problems commanding immediate attention. Solvent technologies for CO_2 capture have become some of the most promising solutions, with aqueous amines being the industrial benchmark system. However, their high regeneration costs render them prohibitive for many of the flue gas applications. The U. S. Department of Energy has invested in the development of different classes of solvents in an effort to reduce parasitic loads and fully deploy these technologies by 2030. In the present talk, synchronized computational, experimental and engineering efforts directed towards the deliberate design of single-molecule, CO_2-bidining organic liquids will be described. The PNNL developed CO_2 capture technology are an attractive alternative to amine-based solvents, but they are plagued by high viscosities at high CO_2 loadings. Using state-of-the-art computational methods and large models we describe the key structure parameters that allowed us to create reduced models for fast screening of potential candidates with low viscosity. Additionally, *ab initio* molecular dynamics and enhanced sampling methods made possible the computation of reaction free energetics for CO_2 binding and proton transfer that control important acid/base equilibrium. Consequently, we were able to make tangible hypotheses towards synthetic targets with appreciable viscosity reductions especially at high CO_2 loadings. These efforts have led to a fundamental understanding of the underlying factors controlling viscosity and the development of several classes of green solvents.

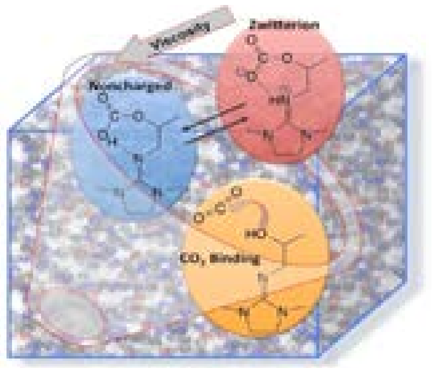

Figure1: Molecular simulation has enabled the discovery of new chemistries resulting in a significant reduction of viscosity in CO_2 capture solvents.

Biography

Vassiliki-Alexandra Glezakou is a Senior Scientist at Pacific Northwest National Laboratory with 20+ years of experience in theoretical/computational methods and simulations techniques. Her research aims towards the understanding, prediction and control of materials relevant to new technologies. Current interests include transition metal chemistry with applications in catalysis and hierarchical materials, materials development for radionuclide remediation, design of CO2 capture and transformation solvents and development of reduced order models to accelerate materials discovery.

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Notes:

Takeo Sasaki, Trends in Green chem, 3:2
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Photo-detachable adhesives composed of photo-depolymerizable poly(olefin sulfone)s

Takeo Sasaki
Tokyo University of Science, Japan

A novel photo detachable adhesive was prepared using a photo-depolymerizable cross-linked poly(olefin sulfone). Poly(olefin sulfone)s containing photobase generators (PBG) are known to exhibit photoinduced depolymerization. A poly (olefin sulfone) is a 1:1 alternating copolymer of an olefin monomer and sulfur dioxide and the protons on the carbons adjacent to the sulfonyl groups in these polymers are readily abstracted by bases. This abstraction results in a depolymerization chain reaction, and so poly(olefin sulfone)s incorporating a photobase-generating chromophore will undergo a photoinduced unzipping reaction. In this reaction, the primary chain of the poly(olefin sulfone) is depolymerized to regenerate the original olefin monomer together with sulfur dioxide. In the present study, a poly(olefin sulfone) composed of a volatile olefin monomer and a second olefin monomer possessing a cross linkable moiety was synthesized. If a mixture of this poly(olefin sulfone) and a crosslinking reagent is sandwiched between glass plates and cured, the plates will be glued together. Subsequently, irradiating the glued plates with UV light in conjunction with heating will separate the plates. In the present study, a poly(olefin sulfone) incorporating carboxylic acid moieties was synthesized and mixed with a polycarbodiimide crosslinker and a photobase generator. The mixture worked as a thermosetting adhesive and exhibited high adhesive strength on quartz plates, comparable to the bond strengths obtained with commercially-available epoxy adhesives. When the bonded quartz plates were exposed to UV light and subsequently heated to 100°C, the poly(olefin sulfone) depolymerized and the plates could be detached.

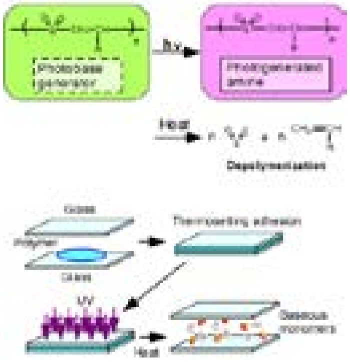

Figure 1: Photoinduced depolymerization of poly(olefin sulfone)s containing photobase generators and a sequence showing a photodetachable thermosetting adhesive.

Biography

Takeo Sasaki is a Professor at the Department of Chemistry, Tokyo University of Science since 2000. He received his Doctorate from the Tokyo Institute of Technology in 1994. He conducts research on Photorefractive Liquid Crystals and Photopolymers. He received the SPSJ Wiley Award (2004) from the Society of Polymer Science, Japan and Senior Membership of SPIE (2016). He is currently a Director of the Japan Liquid Crystal Society and also the Director of the Research Committee on Organic Materials for Information Technology of the Japan Society for Promotion of Science (JSPS).

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Notes:

Joseph F Stanzione III et al., Trends in Green chem, 3:2
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Vanillin: A renewable and versatile platform chemical for sustainable polymers

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[1]Rowan University, USA
[2]Army Research Laboratory, USA
[3]Drexel University, USA

Polymers derived from renewable resources are becoming considerably attractive as sustainable alternatives to their petroleum-derived counterparts. A renewable resource that has gained considerable attention within the past few decades as a viable feedstock is lignin. Lignin is an aromatic biopolymer found in all woody biomass that could yield highly valuable aromatic platform chemicals, including vanillin, when strategically depolymerized. Vanillin, 4-hydroxy-3-methoxybenzaldehyde, is a unique phenolic aldehyde that has been cultivated for flavoring and fragrance for many centuries. However and more recently, with the growing demand to increase our cyclical economy and, thus, improving the planet's overall well-being, vanillin is being utilized as a versatile platform chemical and monomer in the synthesis of a wide range of polymers. This presentation focuses on the history of vanillin in the development of sustainable polymers, including our research efforts in the development and characterization of vanillin-based thermoplastics and thermosets, including epoxies, vinyl esters, polyesters, and polycarbonates.

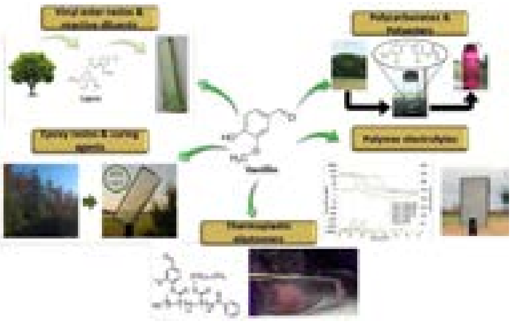

Figure 1: Schematic illustrating the versatility of vanillin in the development of a wide variety of sustainable polymers.

Biography

Joseph F Stanzione III received his MS in Chemical Engineering at Drexel University and his PhD at the University of Delaware under the direction of Professor Giuseppe Palmese and Professor Richard Wool, respectively. He then joined the Chemical Engineering Faculty of Rowan University in 2013. His research program focuses on the utilization of lignocellulosics as an alternative renewable chemicals feedstock; green chemistry and engineering for the development of next-generation lignocellulosic biorefineries; and bio-based polymers and composites for high-performance, biomedical, and energy applications. His work has resulted in one patent, four patent applications, and publications in journals such as *Green Chemistry, ChemSusChem, Journal of Applied Polymer Science and ACS Sustainable Chemistry & Engineering*. Additionally, he is a Co-recipient of US EPA's Presidential Green Chemistry Challenge Award in 2013 and Co-editor of the Special Issue: *Sustainable Polymers and Polymer Science*: Dedicated to the Life and Work of Richard P Wool published by the *Journal of Applied Polymer Science* in 2016.

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Notes:

Dariusz Bogdal, Trends in Green chem, 3:2
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Hydrogen peroxide - Oxidation reactions under microwave irradiation

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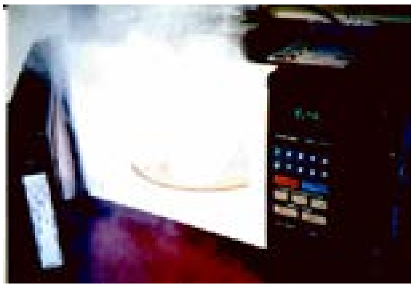
Cracow University of Technology, Poland

In our work, we have successfully used hydrogen peroxide for oxidation of various organic compounds under microwave conditions. First, we considered oxidation of primary and secondary alcohols to corresponding carboxylic acids and ketons as well as N-oxidation reactions. The reactions were performed under phase-transfer catalysis conditions (PTC) in the presence of hydrogen peroxide or urea-hydrogen peroxide complex (UHP) /Na_2WO_4/tetrabutylamonium hydrogensulfate (TBAHS) or hexadecyltrimethyl hydrogensulfate (HDTMHS) as catalysts. Then the reaction systems were modified and hydrogen peroxide encapsulated *in silica* xerogels was applied as oxidizing agent. The xerogel is readily heated by microwave irradiation which could be used as both an oxidizing agent and as solid support for microwave assisted solvent-free oxidation. Finally, Zn-polyoxo-metalated were used as a catalyst; primary and secondary alcohols were oxidized to carboxylic acids and ketones, respectively, in short reaction times (ca. 15 min) under microwave-pressurized conditions. Then, we introduced bromine and chlorine atoms in the halo-oxidation reactions using H_2O_2/HX (HX-hydrohalide acid) system and microwave irradiation. This method, in which bromine and chlorine are generated *in situ* in the reaction of H_2O_2 and HX has several advantages over other bromination/chlorination protocols because whole amount of bromine/chlorine used for a reaction is consumed. Moreover, this system is much easier to handle since bromine transfer and storage facilities are not required. The oxidation of some arenes with the alkyl side groups by means of hydrogen peroxide to corresponding ketones was also investigated. Eventually, we have exploited the method employing the hydrogen peroxide as an oxidant and microwaves irradiation to obtain the epoxy-like compounds from simple alkenes as well as vegetable oils, which in turn we used for the preparation of polyols and polymers. In conclusion, hydrogen peroxide seems to be a very efficient oxidizing agent under the microwave conditions.



Biography

Dariusz Bogdal graduated from Cracow University of Technology (Krakow, Poland), obtained PhD diploma from Jagiellonian University (Krakow, Poland), and Doctor of Science (DSc) diploma from Warsaw University of Technology (Warsaw, Poland). He has more than 30 years of experience in Organic and Polymer Chemistry. He works extensively on the application of phase-transfer catalysis (PTC) and microwave irradiation to organic and polymer synthesis as well as polymer modification. His research interest also includes applying microwave-assisted reactions to polymer chemistry e.g., reactions on polymer matrices, preparation and modification of polymers, preparation and investigation of polymers for dental materials and optical devices. He worked as a Research-Fellow at Clemson University (Clemson, USA), Imperial College (London, UK), Napier University (Edinburgh, UK), and Karolinska Institute (Stockholm, Sweden). He is the author and co-author of books published in Elsevier and Blackwell-Wiley: "*Microwave-assisted Organic Synthesis: One Hundred Reaction Procedures*" (2005) and "*Microwave-enhanced Polymer Chemistry and Technology*" (2007), six book chapters and over 150 papers and review articles.

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Notes:

Youn-Woo Lee, Trends in Green chem, 3:2
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Supercritical fluid technology for greener processes

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Supercritical fluid technology is one of the most promising green chemistry-based future technologies which can develop new, better and clean processes and products. In this presentation, recent R&D activities of supercritical fluid technology are briefly discussed with emphasis on the commercialization efforts. Discussion includes the large-scale (3,000 MT of sesame oil/yr) supercritical fluid extraction (SFE) processes of sesame oil in Korea in which sesame oil contains rich antioxidants like sesamin, sesaminol, and sesamolin. Supercritical CO_2 extraction of residual solvent from Active Pharmaceutical Ingredient (Cefpodoxime Proxetil) preventing unwanted agglomeration of particles will be also discussed. A correlation between the agglomeration phenomenon and dimensionless entropy of fusion (ΔSm/R) was shown on the basis of the hypothesis that CO_2-induced melting point depression is one of the major factors resulting in agglomerates. Other examples of application of supercritical water to wastewater treatment, nano particle synthesis, and recycling of cross-linked polyethylene will be discussed.

Biography

Youn-Woo Lee has completed his PhD in 2004 from Rensselaer Polytechnic Institute, USA. He is a Professor of Seoul National University, Korea. He has over 180 publications and 30 patents. He is a member of Korea National Academy of Engineering since 2014. He has been serving as an Organizer at the International Symposium of Supercritical Fluids 2015, and an Editorial Board Member of the *Journal of Supercritical Fluids and Journal of* CO_2 *Utilization* as well as an Associate Editor of *Green Materials* journal.

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Notes:

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Annalisa Pola et al., Trends in Green chem, 3:2
DOI: 10.21767/2471-9889-C1-002

Graphene-based material for oil spill removal

Annalisa Pola and **Alessandra de Folly d'Auris**
Eni S.p.A, Italy

Oil spill events required efficient and rapid response by authorities and operating staff. The emergency management is not simple and usually is affected by a large consumption of materials and high operative costs. The optimization of the adsorbents is a starting point to reduce these costs. In this study, a graphene-based material (called Grafysorber®, produced by Directa Plus S.p.A) was used inside adsorbent devices (barriers and pillows) to treat waters containing an oily separated phase. Grafysorber® is a super-expanded graphite with a production apparent density of about 2.5 g/L. Three different kind of oils were tested: kerosene, diesel fuel and crude oil, to understand if there is a relationship between viscosity and sorption capacity. In addition, reusability of each device was evaluated. Little pillows of about 10*10 cm were used for adsorption tests. Results showed that the greater is the viscosity, the greater is the amount of oil sorbed; 50.8 g/g for kerosene, 76.5 g/g for diesel fuel, 81.78 g/g for crude oil. Grafysorber® pillows can be reused, after simple squeezing, for about 4-5 times. A progressive decrease of adsorption capacity was detected. Polypropylene, the standard adsorbent material used worldwide in case of water oil spill clean-up activities, showed a sorption capacity at least six times lower than Grafysorber®. The effect of the waves was considered, using diesel fuel, in a 1*5 meters tank, and small adsorbent barriers (7.5 cm diameter and 50 cm length). Water motion caused an increase in the saturation's speed but also an increase of retained water both for Grafysorber® and for Polypropylene barriers. A dropping phase of 5 min is necessary for Grafysorber® and polypropylene devices to favor the water expulsion from the adsorbent device. Anyway, it has been demonstrated that Grafysorber® retains on average the 50% less of water than polypropylene.

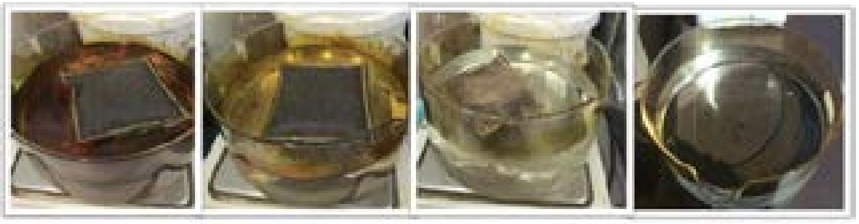

Figure 1: Example of crude oil adsorption by Grafysorber G+

Biography

Annalisa Pola graduated in Environmental Science (University of Insubria – Como – Italy) and is an Environmental Application Manager at Directa Plus S.p.A. Directa Plus is one of the largest producers and suppliers of graphene-based products for use in consumer and industrial markets worldwide.

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Notes:

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Chemical markers for the characterization of bioaerosol

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[2]INAIL, Italy

Bioaerosol is commonly defined as aerosolized particles, with a biological origin, spread into the air by a variety of abiotic and biotic mechanisms. The size of bioaerosol can range from several nanometers to a few hundred micrometres in aerodynamic diameter. Examples of bioaerosols include fungal and bacterial spores/cells, fungal hyphae, pollen, viruses and amoebae, algae, lichen, archaea, aggregates of these particles, and fragments of larger organisms including leaf litter, skin scales, animal and plant debris. Metabolites and excreta are also included in this topic. In these last years the knowledge about indoor and occupational bioaerosol exposure and related diseases has significantly increased. Biological particles have been linked to mucous membrane irritation, allergy, asthma, inflammatory lung diseases, hypersensitivity pneumonitis and so on . The use of biomarkers as a tool for the determination of bioaerosol has often been suggested. The basis of this approach is that bioaerosol components contain chemical compounds that can be used as markers of larger and/or bioactive structures. The main objective of our research is the identification and quantitation of dipicolinic and muramic acids, ergosterol, poliols, amino acids and proteins as markers of bacterial, fungal spores/cells and generic bioaerosol, in both indoor and outdoor airborne particulate matter. To achieve this purpose, methods of extraction and analysis by chromatographic techniques coupled to mass spectrometry of different classes of compounds from particulate matter of different size (ultrafine, fine and coarse), collected in proper sampling campaigns, have been developed.

Biography

Francesca Buiarelli completed her PhD in Chemical Sciences in 1992 and, after several years of work experience, became a Researcher in the field of Analytical Chemistry at Chemistry Department of Rome University "La Sapienza" in 1999. She has been teaching Separative Chemistry since 2002 and has published more than 45 papers in reputed journals. Her research activity involves three main topics: 1) Characterization of polluting agents in airborne particulate matter, water and soil. 2) Excretion study and metabolism of doping agents in sports and veterinary field. 3) Separation and characterization of natural organic compounds in complex matrix such as food.

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Notes:

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Clean and sustainable liquid hydrogen storage materials

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To address the increasing energy and environmental issues, efficient and sustainable energy carriers alternative to carbon based fuels for the current power generation are being extensively investigated. One of the key issues for achieving the "hydrogen economy" is to develop reliable hydrogen storage/release systems that store/release large quantities of hydrogen in a safe and economically viable manner. In this context, liquid organic hydrogen carriers (LOHCs) such as carbazole and methylcyclohexane have attracted significant attention owing to their high reversibility as well as high volumetric hydrogen storage density. In addition to this, carbon dioxide is a potential hydrogen storage medium that can store hydrogen as a form of liquid formic acid (HCO_2H, FA) with a significantly high volumetric H_2 storage capacity of 53 $g.L^{-1}$, much higher than compressed hydrogen gas. Despite the attractive hydrogen release properties of these materials, however, it is still needed to screen highly active and selective catalysts for the reversible hydrogen storage. In this contribution, Pd-based heterogeneous catalysts for FA dehydrogenation are introduced, and relevant H_2-release properties are discussed. Furthermore, liquid organic materials are also proposed as potentially reversible hydrogen energy carriers, and their hydrogenation properties are discussed.

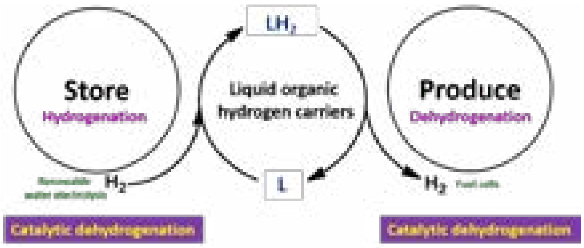

Figure: Catalytic Dehydrogenation

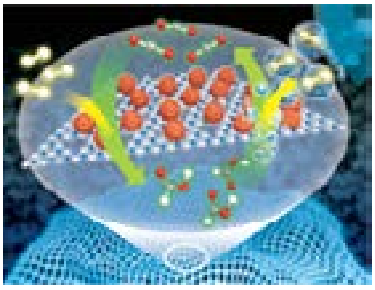

Figure: A schematic image for FA dehydrogenation over Pd/C_3N_4 catalysts]

Biography

Chang Won Yoon is a Principal Research Scientist of the Fuel Cell Research Center at the Korea Institute of Science and Technology (KIST). He is also a Professor of the KHU-KIST Department of Converging Science and Technology at Kyung Hee University as well as a Professor of the KIST School (E&ET). He received his BS and MS in Chemistry at POSTECH in Korea and obtained the Doctoral degree (PhD, 2008) in Chemistry at the University of Pennsylvania (PENN) in USA. He further conducted research associated with Clean Energy in Chemistry at the University of California, Berkeley (2008-2010), and then joined the KIST in 2010. His research has been focusing on hydrogen production and storage particularly for fuel cell technologies as well as on catalysis for a number of chemical transformations related to energy conversion.

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Ahindra Nag et al., Trends in Green chem, 3:2
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Challenges of green chemistry for value added products

Ahindra Nag, **K Mishra** and **H S Maity**
Indian Institute of Technology, Kharagpur, India

Fruit juices and lipases are important applications for the preparation of important value added products such as terpen esters, cosmetics and drug intermediates. Lipases (E.C3.1.1.3) which are highly stereoselective catalysts are used for the resolution of DL menthol by esterification in organic solvent and synthesis of anti-inflammatory drugs in enantiomerically pure form. Glycerol is the by-product of soap industry and has little commercial value which has used for synthesis of 4-methoxy cinnamoyl glycerol (Ultraviolet protecting cream) by lipase in an optimum condition. *Cocos nucifera L. and Borassus flabellifer L.* juices act as bio catalytic system for the reduction of aromatic aldehydes to alcohols and selective decarboxylation of substituted cinnamic acid to styrene and substituted benzoic acid to polyphenolic compound. We have developed a new greener protocol for biotransformation of aromatic aldehydes and acids by fruit juices. The two juices act as solvent, reactant, catalyst and selective to substrate. The purification process of final products is very easy. In this method, protection and deprotection of the phenolic groups are avoided. The reaction system does not use hazardous chemicals. Cucumber juice (CSJ), which acts as a greener solvent system, performing a substrate-selective reaction. Additionally, the hydrolysis of the acetyl as well as the benzoyl group of aromatic compounds has been carried out to afford excellent yield by CSJ. Caffeic acid extracted from potato peel was used for synthesis of caffeic acid amide which has shown antioxidant, clinical drug resistance bacteria and antidiabetic properties.

Biography

Ahindra Nag is currently working as an Associate Professor in Department of Chemistry at Indian Institute of Technology Kharagpur, India. He completed his PhD from Jadavpur University, India. He has 30 years of teaching and research experience in chemistry. He is currently working on natural product isolation and characterization, Bioorganic and Medicinal chemistry. He has published his work in various journals(80) and text books(8). He has guided ten Ph. D students and visited different International universities as a Visiting Professor.

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Diganta Sarma, Trends in Green chem, 3:2
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Waste biomass derived aqueous extracts as alternative green solvent media for organic transformations

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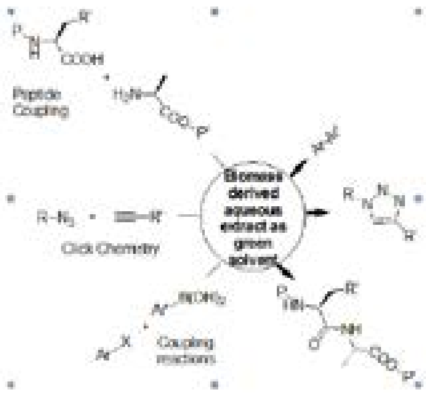
Conventionally most of the organic reactions are carried out in solution phase. The solution phase, that contains pure or mixed solvents, plays a pivotal role in determining the course of reactions and the amount of product formed. The conventional organic solvents used in organic reactions are known to be environment pollutants. In view of the environmental pollution caused by the use of these volatile organic solvents, there is a greater need to replace them by environmentally benign solvents. In this regard aqueous system, ionic liquids, super critical fluids, PEGs have emerged as important substitutes for several organic solvents. Herein, I am presenting how waste biomass derived aqueous extracts can be used as green alternative solvent media for various organic transformations such as Suzuki coupling, click reaction, peptide coupling, etc.




Bananapeels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BSP

Biography

Diganta Sarma is currently working as an Associate Professor in Department of Chemistry in Dibrugarh University, India. He completed his PhD from National Chemical Laboratory, Pune in 2007. He has been a Postdoctoral Research Fellow (2007-2009) at Kyoto Pharmaceutical University, Japan. Worked as Postdoctoral Research Associate, The University of Kansas, USA (2009-12). His research interests include Green Chemistry- Organic transformations (like Suzuki coupling, azide-alkyne cycloadditions, Aza-Michael reactions etc.) in water and ionic liquids, Synthetic Peptide Chemistry/Medicinal Chemistry, Protease inhibitors- Design, synthesis and biological evaluations.

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Water quality of the Chelif River in the Mostaganem area (North-West of Algeria)

Batoul Benkaddour
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This study concerned the water quality of Chelif River, located in the north-west of Algeria which is the most important permanent river of the country. These waters are used for irrigation and drinking water supply. Unfortunately, several towns discharged their wastewater directly into the Chelif River without any treatment which presented a risk for environment and human health. The sampling strategy was based on water samples collected along the watercourse in the Mostaganem area close to the river mouth. One sample was collected on upstream of domestic wastewater discharge point, one sample was collected on downstream of the same domestic wastewater discharge point and one sample was collected close to the river mouth. One sample was also collected directly in the domestic wastewater discharge. Sampling was realized seasonally (February, April, August, and December 2015). All samples were stored in the dark at 4°C before analysis. The physicochemical parameters measured were: pH, conductivity, Chemical Oxygen Demand (COD), Biochemical Oxygen Demand (BOD_5), chloride, nitrates, nitrites, and the total suspended matter (TSM). The urban pollution was monitored through the analysis of tryptophan (tracer of the urban wastewater). The trace metals were also analyzed: Pb, Cu, Zn, Cr, Ni, As and Cd. The urban rejection was characterized by higher concentrations in winter with: COD: 744 mg O_2/l, BOD5: 340 mg O_2/l, Cl^-: 575, 1 mg/l, TSM: 390 mg/l, Cr: 120 µg/l, tryptophan: 5 µmol/l. At the same season, we have observed the impact of the wastewater discharge on the watercourse through the increase of 6.5% of parameter concentrations (COD, BOD_5, Cl^-, Cr) between upstream and downstream of the domestic wastewater discharge. On the other hand, the station located close to the river mouth presented higher values in autumn with: COD: 576 mg O_2 /l, BOD_5: 140 mg O_2/l, Zn: 117 µg/l, Ni: 28 µg/l. The present work allowed to evaluate the impact of anthropogenic pollution on the water quality of Chelif River.

Biography

Batoul Benkaddour is a PhD student in her third year. She prepared her thesis title: “Contribution to the contamination of waters and sediment of Chelif river (Algeria)” between the University of Mostaganem in Algeria and the University of Perpignan in France. She carried out this research to evaluate the water quality of the Chelif river, the greatest watercourse in Algeria. The present work is included in the framework of the improvement of the Chelif’s water quality, which is used for drinking water supply and irrigation. The obtained results allowed alerting the responsibility to implement water treatment systems before discharging wastewaters in watercourse.

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Notes:

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Global atmospheric emissions of toxic heavy metals from anthropogenic sources under multi-scale regions

Hezhong Tian and **Chuanyong Zhu**
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Based on economic development and technology diffusion theory, anthropogenic atmospheric emission of typical heavy metals (HM, Hg, As, Se, Pb, Cd, Cr, Ni, Sb, Mn, Co, Cu and Zn) characterized by global multi-scale regions, long-term spans and high spatiotemporal resolutions were established by synthetically using the best available representation of time-varying emission factor methods and ArcGIS tools. The main conclusions are summarized as follows: Emissions of 12 toxic heavy metals in China during the period of 1949-2012, increased by about 20-128 times, totally reaching about 79807.7 tons in 2012, and contributing 36.8% of global emissions (about 216893.1 tons). Coal combustion, liquid fuel combustion, nonferrous metal smelting and brake wear were identified as the primary sources for the corresponding heavy metals. Generally, Shandong (for As, Se, Cd, Cr, Ni, Sb and Cu), Hebei (for Pb and Zn), Guizhou (for Hg), Inner Mongolia (for Mn) and Shanxi (for Co) ranked as the largest provinces, respectively. Emission intensities of HMs were much higher in central and eastern China than those in western China, and the coastal regions were classed as the most polluted areas of varied HMs. Worldwidely speaking, China, Chile, India, Russia, the United States and South Africa are the countries with high HMs burden. Therein, China ranked as the top one largest country with HMs (except for Sb) emissions. Asia represented the highest heavy metals emitting continent, which accounts for approximately 58.6% of the global emission in 2012. The top emission intensities of HMs were found in Eastern and Southern Asia and Eastern Europe.

Biography

Hezhong Tian has completed his PhD from Tsinghua University and Postdoctoral Studies from Tsinghua University School of Environment. He is now the Director of Center for Atmospheric Environment Studies, Professor of School of Environment at Beijing Normal University of China. He has published more than 50 papers in reputed journals like ES&T, and ACP, and has been serving as an Editorial Board Member of *Environmental Science Studies*.

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Notes:

S M Contreras-Ramos et al., Trends in Green chem, 3:2
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Removal of oil hydrocarbons using the grass *Panicum maximum* and a bacterial consortium in contaminated soil

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[2]Universidad Veracruzana, Mexico
[3]Instituto de Ecología A.C., Mexico

The phytoremediation is a bioremediation technology used for the contaminants removal in soil and plants of tropical areas which has showed their potential with oil hydrocarbons. Species of grass belonging to *Panicum* genus has been found in oil contaminated soil. In this study, the aim was evaluating the removal of oil hydrocarbons from soil using the grass *Panicum máximum* alone or combined with a bacterial remover consortium. Grass and oil contaminated soil were collected from a closed oil extraction field and greenhouse experiment was established with consortium Bacterial (B), Grass (G) and their combination (G+B) on soil-cow manure-agrolite (1.8:0.1:0.1 w/w) in sterilized and not sterilized treatments during 112 days. A control (natural attenuation) without treatment was established in same conditions. Bacterial consortium was selected and mixed to growth as consortium after encapsulated with liposome in a permeable matrix of sustained release. The height, number of leaves, *total hydrocarbon concentration* (TPH) was recorded at 0, 28, 56 and 112 days, and grass biomass (root and steam) was determined at the end. TPH was determined by GC-MS. The treatment with only grass has a significant growth after 28 days up to end of the experiment, presented significantly higher root biomass than other treatments. The higher oil hydrocarbons removal was observed in the treatment of bacterial consortium (85%) followed by combined G+B (80%) and grass (77%) than natural attenuation (15%). The bioaugmentation with bacterial potentialized the oil hydrocarbons removal and helped the phytoremediation using the grass *Panicum máximum*.

Biography

S M Contreras-Ramos has completed her PhD from Centro de Investigación y Estudios Avanzados del IPN (CINVESTAV) and Postdoctoral studies from Universidad Autónoma de México (UNAM). She is now the Director of Environmental Technology Unit in CIATEJ, and received Prize of Innovation 2016 grant by Jalisco Government State. She has published more than 25 papers in recognized and international journals reaching 400 cites (no self-citations), h-index=12 and has been serving as an Editorial Review Member of reputed international journals.

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Scientific Tracks & Abstracts

Day 3

Green Synthesis | Green Manufacturing | Green Chemistry

Session Chair
Ettigounder Ponnusamy
Millipore Sigma, USA

Session Co-Chair
Antonio Zuorro
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Session Introduction

Title: DOZN – A quantitative green chemistry evaluator
Ettigounder Ponnusamy, Millipore Sigma, USA

Title: Production of silver nanoparticles by spent coffee grounds extracts
Antonio Zuorro, Sapienza University of Rome, Italy

Title: Asymmetric synthesis of potential biologically active new heterocyclic analogs of (s)-α-alanine containing 3,4-substituted 5-thioxo-1,2,4- triazoles in the side-chain radical
Hayarpi M. Simonyan, Yerevan State University, Armenia

Title: Innovative green routes to noble metal nanoparticles
Magda Blosi, Institute of Science and Technology for Ceramics, Italy

Title: Efficient method for the synthesis of novel enantiomerically enriched derivates of propargylglycine
Anna F. Mkrtchyan, Yerevan State University, Armenia

Title: Micro/nano-architecture assisted electrochemistry on electrode materials Bioinspired by butterfly wings
Tongxiang Fan, Shanghai Jiaotong University, China

Title: Ultrasound and microwaves assisted synthesis of molecules with antiquorum sensing activity
Alicia Reyes-Arellano, National Polytechnic Institute, Mexico

Title: Mimetic peptides based on promiscuous enzyme as asymmetric catalyst in Aldol and Michael reactions
Saadi Bayat, Tofigh Daru Research and Engineering Company, Iran

Ettigounder Ponnusamy, Trends in Green chem, 3:2
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DOZN – A quantitative green chemistry evaluator

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Millipore Sigma created a unique web-based greener alternative scoring matrix, also known as DOZN™, a quantitative green chemistry evaluator based on the 12 principles of green chemistry. The 12 principles of green chemistry provide a framework for learning about green chemistry and designing or improving materials, products, processes and systems. DOZN scores products based on metrics for each principle and aggregates the principle scores to derive a final aggregate score. The system calculates scores based on manufacturing inputs, GHS and SDS data which provide a green score for each substance. DOZN is flexible enough to encompass the diverse portfolio of products ranging from chemistry to biology based products. The DOZN system has also been verified and validated by a third party to ensure best practices and are applied. This new greener chemistry initiative offer customers an increased breadth of greener alternative products with confirmatory documentations to validate greener characteristics.

Biography

Ettigounder Ponnusamy completed his PhD at the University of Madras (India) in 1982 and Postdoctoral studies at the University of Illinois at Chicago (1983-87). In 1988, he joined Sigma-Aldrich as an R&D Scientist and worked on many high value projects at various capacity. Currently he is the Fellow in Green Chemistry at MilliporeSigma (formerly Sigma-Aldrich), leading the Green Chemistry Initiatives. His work was recognized by The Academy of Science St. Louis, and awarded an Outstanding Scientist Award in 2011 and also inducted as a Fellow of the Academy of Science St. Louis.

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Antonio Zuorro et al., Trends in Green chem, 3:2
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Production of Silver Nanoparticles by spent coffee grounds extracts

Antonio Zuorro, Gianluca Maffei, Annalaura Iannone and **Roberto Lavecchia**
Sapienza University of Rome, Italy

Spherical silver nanoparticles (AgNPs) were synthesized through a novel green method employing spent coffee grounds (SCG) phenolic extracts obtained with hydro-alcoholic mixtures. The bio-reduction of AgNPs was carried out at 25 °C under stirring, employing an aqueous solution of silver nitrate as a precursor and the polyphenols obtained from SGC extracts as reducing and capping agents. To monitor the formation of AgNPs, UV-Vis spectra were recorded and the intensity of the surface plasmon resonance (SPR) band of silver at 405–430 nm was measured. The synthesis of Ag NPs was completed in 5 hours. Trasmission Electron Microscopy (TEM) observations showed that the AgNPs obtained exhibited a spherical shape. The mean hydrodynamic diameter and zeta-potential were measured through Dynamic Light Scattering (DLS) technique. XRD patterns were acquired to assess the crystalline structure of the AgNPs, which exhibited a cubic face centered lattice.

Figure: Appearance of the reaction mixture (silver nitrate solution and 50% aqueous ethanol extract from SCG) after 3 hours.

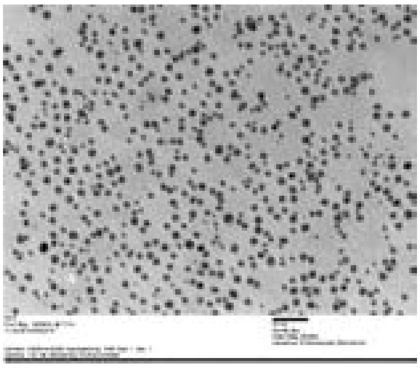

Figure: TEM imaging of AgNPs

Biography

Antonio Zuorro is working as an Assistant Professor of Chemical Engineering Fundamentals at the Department of Chemical Engineering Materials & Environment of Sapienza University of Rome, where he received his M.S. and Ph.D degrees in Chemical Engineering. His research activity has been mainly focused on the development of innovative chemical and biotechnological processes for the recovery of high value-added compounds from by-products and agro-industrial residues, such as lycopene from tomato waste and phenolic antioxidants from artichoke and bilberries waste, olive pomace and coffee grounds. He also examined the possibility of including the extracts obtained in consumer food products to get new functional foods with high antioxidant activity. In the field of enzyme technology, he studied the use of multienzyme systems with enhanced activity for the recovery of lipids and bioactive compounds with high added value from microalgae. He is the author of over 60 scientific publications and also co-author of five industrial patents.

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Asymmetric synthesis of potential biologically active new heterocyclic analogs of (S)-α-alanine containing 3,4-substituted 5-thioxo-1,2,4- triazoles in the side-chain radical

Hayarpi M Simonyan[1,2], **Lusine Yu Sahakyan**[1,2], **Anna F Mkrtchyan**[1,2], **Satenik Gh Petrosyan**[1,2], **Narine N Baghyan**[3], **Ani O Voskanyan**[3], **Jaklina N Saribekyan**[3] and **Ashot S Saghyan**[1,2]
[1]Yerevan State University, Armenia
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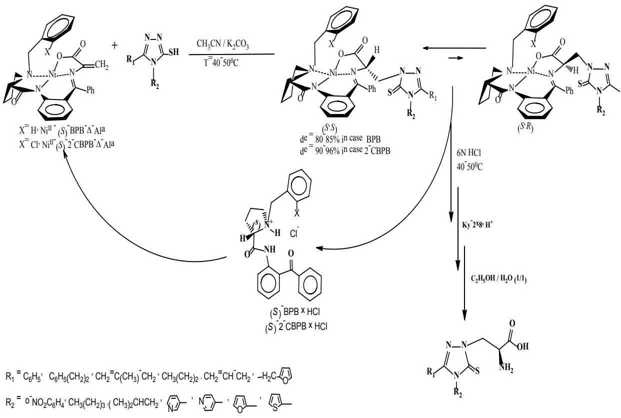
Statement of the Problem: Non-proteinogenic α-amino acids are constituents of many physiologically active peptides, antibiotics and other pharmaceutical preparations. Especially α-amino acids and peptides, containing a N-heterocyclic substituent in the side chain, are of considerable importance in medicinal chemistry because they combine the pharmacophoric groups of amino acids and N-heterocycles. These compounds also belong furyl-, thiophenyl- and triazole-containing structures that are important constituents of many biologically and pharmacologically active drugs such as anti-hyperglycemic, analgesic, anti-inflammatory, antibacterial, anticancer, antifungal, antitumoral, antiviral and psychotropic.

Aim: The goal of our research work is elaboration of efficient high-selectivity method for asymmetric synthesis of enantiomerically enriched substituted α-alanine containing triazole rings in side chain radical.

Materials & Methods: Efficient high-selectivity method for asymmetric synthesis of new heterocyclic substituted derivatives of α-alanine, through the nucleophilic addition of the substituted triazoles to the C=C bond of dehydroalanine moiety in NiII complexes of Shiff's base with chiral auxiliaries (S)-2-N-(N'-benzylprolyl)aminobenzophenone and (S)-2-N-(N'-chlorbenzylprolyl) aminobenzophenone was elaborated.

Results: The results show, that the stereoselectivity of the reaction of nucleophilic addition in case of the complex containing Cl-atom at the 2nd position of Ph-group of N-benzyl proline moiety is increased (up to 96%). Heterocyclic substituted derivatives of (S)-α-alanine were isolated with high optical purity (ee>99%) after decomposition of the mixture of the diastereomeric complexes and ion-exchange purification of the target amino acids.

Conclusion: The advantage of these complexes is the regenerability of the initial chiral auxiliary reagents in quantitative chemical yield and complete retention of the original chirality (optical activity) after completion of the synthesis and isolation of the desired products. This allows multiple reuses of the chiral auxiliaries.



Biography

Hayarpi M Simonyan works in Institute of Pharmacy of Yerevan State University. Her research field of interest is Biomimetic Asymmetric Synthesis. She has her expertise in elaboration of high selective methods of asymmetric synthesis of enantiomerically enriched non proteinogenic amino acids. She completed her PhD degree in Chemistry during the year 2013 specializing in Bioorganic Chemistry.

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Anna F Mkrtchyan et al., Trends in Green chem, 3:2
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Efficient method for the synthesis of novel enantiomerically enriched derivatives of propargylglycine

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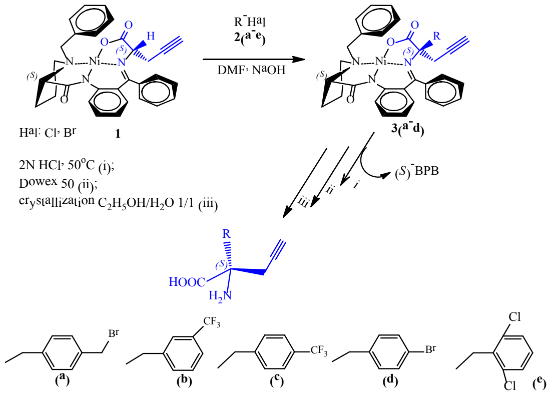
Alkyne-containing amino acids are versatile structures readily available by a number of methods and are accessible using very few transformations from economical starting materials. They can be functionalized by many chemical functions and offer a wide range of possible transformations. Particularly, unsaturated α-amino acids give access to many synthetic applications in all fields of chemistry. Among them, metal catalyzed cross-coupling reactions and cross metathesis are commonly used to generate peptide modifications and cyclization. They are very interesting and useful tools for “Click” Chemistry in peptidomimetic drug design or covalent modification of proteins. They can also be incorporated in compounds as beta-turn inducer to promote secondary structures. Finally they can be used for the preparation of stapled peptides. Some such amino acids are commercially attainable in enantiomerically pure form. Here, we present a stereoselective approach to synthesize unsaturated α-amino acids in optically active form. As a starting amino acid synthon for the asymmetric synthesis of amino acids NiII square-planar complexes of Schiff’s bases of propargylglycine with chiral auxiliary (S)-2-N-(N`-benzyl-prolyl)aminobenzophenone (BPB) (1) was taken. As a result effective methods of asymmetric synthesis for novel enantiomerically enriched derivatives of (S)-propargylglycine (S)-propargylglycine (ee > 80%) was developed.



Biography

Anna F Mkrtchyan works in Institute of Pharmacy of Yerevan State University and SPC “Armbiotechnology” NAS RA. She got her PhD degree in Chemistry in 2013 specializing in Bioorganic Chemistry.

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Notes:

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Tongxiang Fan et al., Trends in Green chem, 3:2
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Micro/nano-architecture assisted electrochemistry on electrode materials bioinspired by butterfly wings

Tongxiang Fan and **Xingmei Guo**
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Rapid depletion of fossil fuels raises serious energy and environmental problems. Electrochemistry which converts chemical energy into electrical energy/signal with little or no pollution is a more sustainable and environmentally friendly way to support the fast developing world. Researching and developing efficient electrode materials is a basic and essential issue to promote electrochemical performance in almost all electrochemical devices. Due to its high specific surface area, micro/nano architectured electrodes are increasingly investigated and studied. In the past few years, our group use butterfly wings as template warehouse to obtain electrode materials with various elaborate micro/nano-architectures and explore architecture effects on different electrochemical systems. Pt samples with three different butterfly-wing architectures were synthesized through electroless deposition and investigated as anode materials for methanol oxidation. Lamellar ridge-Pt was proved to exhibit the best electrocatalytic performance, whose methanol oxidizing peak current density was 5.2 times higher than its unarchitectured counterpart. This work confirms the lamellar ridge butterfly-wing architecture as one of the most effective electrode architectures, which shows great application potential in the electrochemical arena. To extend application arena to electrochemical detection, lamellar ridge-Au was fabricated using the same method. The sensitivity for glucose electrochemical detection was increased by 5.8 times and the detection limit was lowered by 3.7 times compared to its unarchitectured counterpart. According to simulation results, an efficient zigzag diffusion in the lamellar-ridge architecture and more efficient "thin layer diffusion" in the space of adjacent lamellae occurred for rapid transport and depletion of electrolytes. By combining experimental and simulation method, these efforts provide a simple and reliable way to select efficient micro/nano-architectures for electrode based on the structural pool of butterfly-wings. These efforts may provide reference and prototype for future structural design of electrode materials with enhanced electrochemical performance.

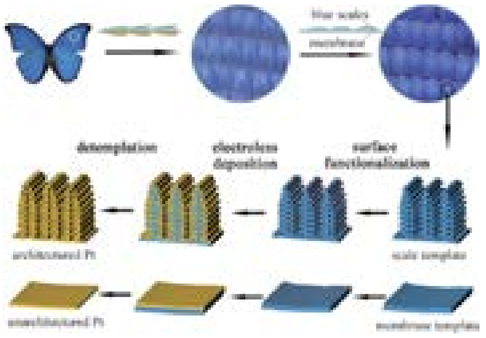

Figure 1: Schematic diagram of the preparation process of architectured Pt and unarchitectured Pt using lamellar-ridge architectured blue scales and flat membrane from Morph butterfly wings as sample templates through surface functionalizing, electroless deposition, and detemplating procedure.

Biography

Tongxiang Fan received his PhD in Materials Science from Shanghai Jiaotong University in 1999. He is currently a Professor of Materials Science in Shanghai Jiaotong University, China. He has received several scientific awards, including the STA Fellowship (Japan, 2000) and Fok Ying Tung Foundation (Hong Kong, 2003). His main research interests focus on bioinspired/biomimetic materials and their applications in energy and environmental fields.

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Alicia Reyes-Arellano et al., Trends in Green chem, 3:2
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Ultrasound and microwaves assisted synthesis of molecules with antiquorum sensing activity

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Statement of the Problem: It is necessary to synthesize molecules that can function as biososteres[1] of acyl homoserine lactones[2] (AHL) or bioisósteres of tirosol,[3] which can be evaluated on Gram-negative bacteria or Candida albicans respectively. On the other hand it is indispensable that the synthesis is carried out considering energy efficiency, operational simplicity and good yield in short times. By the above mentioned, molecules were designed for this purpose and planted some chemical synthesis procedures.

Findings: Compounds 1 were synthesized in two steps, from p-hidroxy benzaldehyde,[4] one of them was carried out by sonication. Compounds 2 were totally synthesized by sonication, based on a report of literature[5]; global isolated yield 85-95%. Synthesis of compounds 3 and 4 involves a cyclization, it was carried out by MW or ultrasound. Good yields were obtained when the raw material contain long chains. Excellent yields were achieved when the raw material had short chains. The ultrasound has the advantage the time is minimum compared with MW or conventional heating. Compounds 3 were prepared from p-amino toluene and compound 4 from p-hydroxibenzaldehyde. It is important to mention that alkylation of p-hydroxibenzaldehyde demands 18h of heating, while using MW the reaction requires only 4h and 2h with ultrasound.

Conclusion & Significance: Diols, alcohols and imidazolines were prepared using a very simple protocols using MW or ultrasound in good to excellent yields. The synthesized compounds are currently evaluated as antiquorum sensing molecules in Serratia marcescens and Candida albicans, in fact some of them present activity as antiquorum sensing compounds.

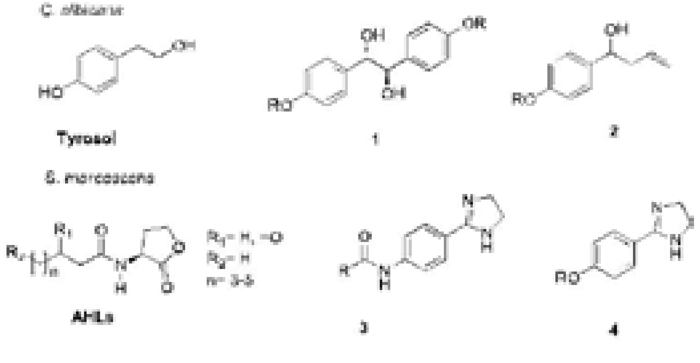

Figure 1. Tyrosol, autoinductor or semiochemical of *Candida albicans*. AHLs, Acyl homoserin lactones, autoinductors of *Serratia marcescens*. Compounds 1, bioisosteres of tyrosol. Compounds 2-4 bioisosteres of AHLs

Biography

Alicia Reyes-Arellano has her expertise in design and synthesize of compounds with pharmacological activity and passion in improving the synthetic procedures according the green chemistry. Her fields are organic chemistry, medicinal chemistry and nanostructures synthesis. She has interest in teaching and improved the plans and curricula in her Institution. She is also interested on HPLC-MS studies

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Saadi Bayat et al., Trends in Green chem, 3:2
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Mimetic peptides based on promiscuous enzyme as asymmetric catalyst in Aldol and Michael reactions

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[2]Tofigh Daru Research and Engineering Company, Iran

Biocatalysis has emerged as an elegant and green tool for modern organic synthesis due to its high efficiency, good selectivity and environmental acceptability. Although, an enzyme is capable of catalyzing a specific reaction effectively, some unexpected experimental results have indicated that many enzymes are catalytically promiscuous. Mimetic peptides based on enzyme as a kind of important chiral scaffold are broadly identified for their obvious advantages, diverse structures and ready accessibility. Based on promiscuous aldo-keto-reductase enzymes, several mimetic peptides were designed which were synthesized and tested as multifunctional organocatalysts in direct asymmetric aldol and Michael reactions. The asymmetric aldol and Michael reactions, as the most prominent carbon-carbon bond formation reactions, are the central study issues in the field of asymmetric synthesis. In this study, promiscuous aldo-ketoreductase (AKR) is used to catalyze aldol reaction between aromatic aldehydes and ketones. Good yield (up to 75%), moderate enantioselectivity (60%), and high diastereoselectivity (dr) up to 93/7 (anti/syn) were obtained. Several mimetic peptides from AKR's active site were designed and synthesized as asymmetric catalysts in the aldol and Michael reactions. The corresponding aldol products were produced with high yields (up to 97%) and excellent diastereoselectivities (up to 99/1) and enantioselectivities (up to 99.9) under mild reaction conditions. These peptides exhibit excellent catalytic activity in terms of yield, diastereoselectivity and enantioselectivity. The secondary structures of peptide catalysts provide an understanding of their mechanism.

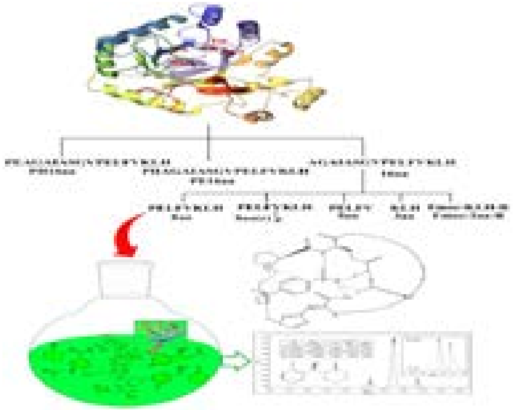

Figure 1: Synthesized mimetic peptides as asymmetric organocatalyst

Biography

Saadi Bayat received his BSc in Applied Chemistry at Buali Sina University (Hamedan, Iran, 2000). He completed his Postgraduation with MSc in Organic Chemistry at Kharazmi University (Tehran, Iran, 2008). He had enrolled in PhD program at Department of Chemistry, Faculty of Science of University of Putra Malaysia (UPM), under supervision of Prof. Dr. Mohd Basyaruddin Abdul Rahman. The following year, he was offered scholarship from Graduate Research Assistance (GRA), UPM. Moreover, his research program focuses on mimetic peptide as asymmetric catalysis. He employed strategies that include organo-catalyst design, and the application of these approaches to construct asymmetric C-C bond forming and esters hydrolysis. He was as a Postdoctoral Research Fellow for a year (May 2014-June. 2015) in UPM. He has been selected to receive Endeavor scholarship from Australian Government and has joined Dr. Bellinda Abott in La Trobe University, Melbourne (July 2015-January 2016).

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Notes:

Sessions

Day 3 July 26, 2017

Renewable Sources | Non-thermal Activation Methods | Valorisation of Waste into Chemicals

Session Chair
Detlef Schmiedl
Fraunhofer Institute for Chemical Technology, Germany

Session Co-Chair
Manuel Garcia-Perez
Washington State University, USA

Session Introduction

Title: Potential deconstruction of recycled wood, structural features of isolated lignin and ways to activate it for material applications

Detlef Schmiedl, Fraunhofer Institute for Chemical Technology, Germany

Title: Bio-oil refineries: Challenges and opportunities

Manuel Garcia-Perez, Washington State University, USA

Title: Use of clays and clay wastes as artificial pozzolans in eco-cement manufacture: A review

Siline Mohammed, University of M'sila, Algeria

Title: Research on antidote of cyanidepoison(sodium & hydrogencyanide) known as Sodasulphanecoblamin

Salako Olatunji, FIIRO & ACS Chemistry Ambassador, Nigeria

Young Researchers Forum

Title: Synthesis of a stable iron oxide nanoparticles in ionic base fluid for photo-thermal conversion applications

Ehsan Nourafkan, University of Leeds, UK

Title: Biomass nitrogen-enriched pyrolysis for nitrogen-doped carbon materials of supercapacitors

Wei Chen, Huazhong University of Science and Technology, China

Title: Green design of lock-and-key affinity devices to address API purification challenges

Raquel Viveiros, Universidade NOVA de Lisboa, Portugal

Title: Valorization of lignocellulosic biomass and production of biofuel precursors under microwave radiation

Almudena Lorente, University of Castilla La Mancha (UCLM), Spain

Title: Chemoselective hydrodehalogenation and high efficiency birch reduction using two-dimensional inorganic electride dicalcium nitride ($[Ca_2N]^+\cdot e-$) as a reducing agent

Byung Il You, Sungkyunkwan University, Republic of Korea

Title: The new class of green material: Two-dimensional electride $[Ca_2N]^+\bullet e^-$

Ye Ji Kim, Sungkyunkwan University, Republic of Korea

Title: Phytoremediation of heavy metal-polluted aquatic ecosystem (ologe lagoon) by water hyacinth (eichhornia crassipes [mart.] solms) and the socio-ecological implications

Isreal Ugochukwu Oshiojum, Lagos State University, Nigeria

Title: Reusable cobalt-phthalocyanine in water: Efficient catalytic aerobic oxidative coupling of thiols to synthesize organosulfur compounds

Bingxin Yuan, Zhengzhou University, China

Title: Removal of a tar analogue from synthetic fuel gas using a non-thermal plasma dielectric barrier discharge reactor

Faisal Saleem, Newcastle University, UK

Title: Design and elaboration of MV_2O_6 nanomaterial with different synthesis methods: Impact on structure and catalytic properties

Khadija Khallouk, Université de Montpelier, France

Detlef Schmiedl et al., Trends in Green chem, 3:2
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Potential deconstruction of recycled wood, structural features of isolated lignin and ways to activate it for material applications

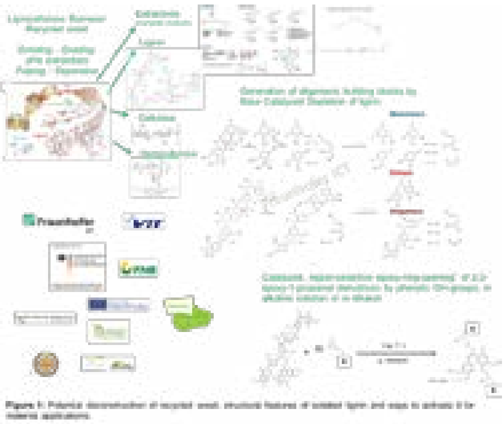
Detlef Schmiedl[1], **Jürgen Graf**[1], **Beatrice Tübke**[1], **Tiina Liitiä**[2], **Anna-Stiina Jääskeläinen**[2] and **Matti Siika-aho**[2]
[1]Fraunhofer Institute for Chemical Technology, Germany
[2]VTT Technical Research Center, Finland

Statement of the Problem: With global rising use of wood & other lignocelluloses in the future, the importance of efficient utilization of recycled wood (RW) will increase. Present utilization ways of RW-AI (natural wood, only processed mechanically, German classification) are composites & combustion. Composition and availability of RW-AI offer a high potential for valorizing in biorefineries to generate biogenic chemicals & fuels. The efficiency of present & future lignocellulose biorefineries can be increased by valorizing of lignin.

Methodology: A potential decomposition process of RW-AI is ethanol based E/W-OrganoSolv cooking to generate well hydrolysable polysaccharides & Sulfur-free lignin. Depending on parameters, high quality lignin charges, differing in yield & features (MN, MW, MW/MN, phenolic & aliphatic OH-groups) are available. It is evident, that valorizing of lignin in several material applications strongly depends on present & on adjustable structural features by chemical modification. Such lignin activation steps are: grafting of molecules, containing defined functional groups (e.g. 2, 3-epoxy-1-propanol & derivatives), onto the lignin-based molecule, as well as catalyzed generation of oligomers, with accompanying elimination of steric hindrances & increase in phenolic OH-groups.

Findings: Optimized auto- & acid-catalyzed E/W-OrganoSolv on RW-AI generate lignin yields of 50 to 70% respectively, in high quality & charges differing in structural features. Base Catalyzed Depletion (BCD) of lignin in a continuously plug flow reactor, under gentle to strong conditions, generate BCD-oligomers with yields of 90 to 40% respectively. Structural features of lignin & of oligomers are adjustable. The addition reaction, "catalyzed, region-selective epoxy-ring-opening" of 2, 3-epoxy-1-propanol by phenolic OH-groups, in alkaline solution or in ethanol is useful to increase the aliphatic OH number in lignin & BCD-Oligomers. Several catalysts are available to use also green solvents, as reaction medium.

Conclusion: Such lignin modification processes enlarge the scope of application as a result of changes involved in chemical & physical characteristics.



Biography

Detlef Schmiedl, PhD, has his expertise in bioeconomy, lignocellulose biorefinery and chemical modification processes of macro molecules, like lignin, with the target to develop and to illustrate process parameter effects on structural features, structure-function-relationships and catalyzed chemical modification path ways. His passion is to develop environmental friendly, chemical processes according to the principles of green chemistry.

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Manuel Garcia-Perez et al., Trends in Green chem, 3:2
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Bio-oil refineries: Challenges and opportunities

Manuel Garcia-Perez, Filip Stankovikj and **Iva Tew**
Washington State University, USA

Biomass derived pyrolysis oils are complex mixtures of hundreds of compounds. These oils typically contain water (19-26 wt.%), GC/MS detectable volatile compounds (30 wt.%), lignin derived oligomers (15-23 wt.%) and water soluble (WS) compounds (28-36 wt.%). The nature of the WS oligomers is still poorly known. In this presentation, we will discuss two strategies to describe the bio-oil composition in terms that can be used for engineering design. The first approach is formalization of the bio-oils' composition in terms of functional groups; the second describes bio-oils' composition in families based on their volatility behavior in thermogravimetric analyses. The chemical composition of the WS fraction is described in detail. Our FT-ICR-MS and UV-Fluorescence studies allowed us to identify the presence of two new fractions: dehydrated sugars and WS oligomeric phenols. Here we will discuss the advances made by our group on the evaluation of bio-oil new separation schemes and on the development of new products from bio-oil fractions. The combination of these separation schemes with technologies to obtain high value products is foundation for the synthesis of new bio-refinery concepts. We will address several potential bio-refinery concepts, their challenges and opportunities.

Biography

Manuel Garcia-Perez is an Associate Professor for the Biological Systems Engineering Department at Washington State University. He has been working for the last 15 years on projects related with the thermochemical conversion of lignocellulosic materials for the production of bio-fuels and chemicals. So far he has published more than 110 peer reviewed papers. He has made contributions to the understanding of thermochemical reactions of cellulose and lignin as well as the characterization and uses of crude bio-oils. He is currently working on the development of more selective pyrolysis reactors and on new concepts to refine pyrolysis oils. He is also very active on the development and characterization of engineering carbonaceous materials.

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Day 3

Ehsan Nourafkan et al., Trends in Green chem, 3:2
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Synthesis of a stable iron oxide nanoparticles in ionic base fluid for photo-thermal conversion applications

Ehsan Nourafkan and **D Wen**
University of Leeds, UK

Microemulsion-mediated method is one of the unique and ideal techniques for the preparation of nanoparticles. A one-pot microemulsion method was introduced in this research to synthesize and disperse iron oxide (Fe_3O_4) in an ionic base fluid of lithium bromide-water. An effective steric repulsion force was provided by the surface functionalization of nanoparticles during the phase transfer. The functionalization stage was performed by formation of a bi-ligand surfactant around nanoparticles during the phase transfer of particles from oil phase to water phase. The formed nanoparticles exhibited a superior stability against agglomeration in the presence of high concentrations of lithium bromide, i.e. 50 wt%, which make them good candidates for a range of novel applications. The nanoparticles were analyzed by zeta potentiometer, Lumisizer dispersion analyzer, UV-visible spectroscopy, dynamic light scattering (DLS) and transmission electron microscopy (TEM). As the reactants concentration and temperature is elevated, the crystalline structure completion increase gradually, and the morphology of nanoparticles changes from a spherical into a rod-like shape. The photo-thermal conversion characteristics of spherical and rod-shape nanoparticles also was studied under a solar simulator. Experimental analysis indicates that the benefit of adding iron oxide nanoparticles into fluid was not only increasing photon trapping efficiency to increase the bulk temperature under solar radiation, but also more likely to increase evaporation rate due to surface localized heat generation. According to the results, the suitable photo-thermal conversion of nanoparticles together with high stability in ionic media, nominates the iron oxide nanoparticles as a good candidate for using in solar air conditioners.

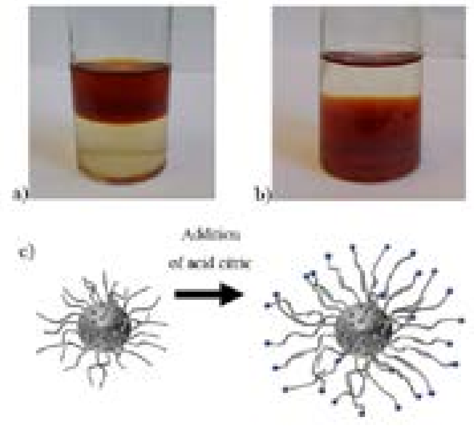

Figure 1: (a, b) phase transformation of iron oxide nanoparticle from organic phase to aqueous phase, and (c) the proposed mechanism for formation new ligand around particles during phase transformation.

Biography

Ehsan Nourafkan is a Research Fellow in the School of Chemical and Process Engineering at the University of Leeds. His research interests are Surface Chemistry, Polymers and Colloid Science, Nanofluids and Green Energy.

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Notes:

Haiping Yang et al., Trends in Green chem, 3:2
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Biomass nitrogen-enriched pyrolysis for nitrogen-doped carbon materials of supercapacitors

Haiping Yang, Wei Chen, Yingquan Chen, Mingwei Xia, Xu chen and **Hanping Chen**
Huazhong University of Science and Technology, China

Biomass is a clean, renewable and abundant resource that can be converted to bio-char, bio-oil and fuel gas through various thermochemical processes. Conversion of biomass for high value products is an important development direction for biomass utilization, which has attracted more attention. In this study, a new method of biomass pyrolysis with exogenous nitrogen introduced was proposed. The influence of NH_3 on the property of bamboo pyrolysis process and products characteristics was investigated with variant approaches (e.g. elemental analysis, automatic adsorption equipment, X-ray photoelectron spectroscopy and CHI760 electrochemical workstation) and as well as the influence of KOH (as activator). The results showed that, the specific surface area, the content of nitrogen and nitrogen-containing functional groups of bio-char increased significantly with NH_3 introduced in. On the other hand, with the addition of KOH, the yield of bio-char increased obviously and it increased gradually with increasing KOH amount, and the specific surface area increased dramatically to 1873.17 m2 g-1. The content of nitrogen in bio-char increased greatly with KOH introduced in, especially the content of pyridinic-N and pyrrolic/pyridone-N, while it decreased slightly with increasing KOH amount, but nitrogen content was still relative high (9.1-10.4 wt.%). The formation mechanism of nitrogen-containing functional groups was proposed. Besides, electrochemical analysis showed that the specific capacitance of bio-char electrodes increased with increasing KOH content, and the largest specific capacitance could reach to 187 F g^{-1} at 1 A g^{-1} with good cycling stability. Therefore, it could be concluded that biomass nitrogen-enriched pyrolysis was a promising method for more efficient utilization of biomass resources.

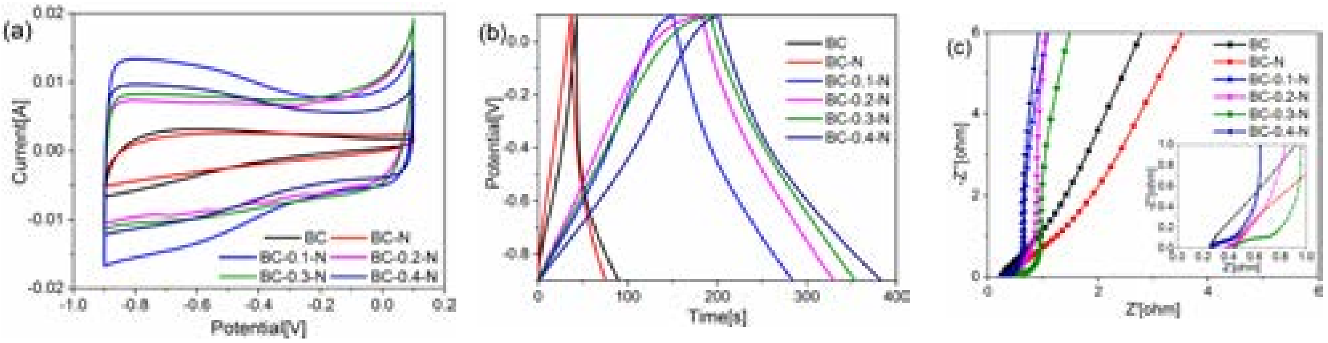

Figure 1: Electrochemical performance of bio-chars: (a) Cyclic voltammetry curves at 10 mV s-1; (b) Galvanostatic charge/discharge curves at 1 A g-1; (c) Nyquist plots (the inset shows the expanded high frequency region of the plot).

Biography

Haiping Yang has been the Research Fellow of the State Key Laboratory of Coal Combustion in Huazhong University of Science and Technology since 2005. She received her PhD degree from Huazhong University of Science and Technology in 2005. Her major research areas are: biomass pyrolysis for gas, bio-oil and char multigeneration, especially on the fundamental study of biomass pyrolysis; Biomass gasification for H2 enriched synthesis gas; Biomass catalytic fast pyrolysis for liquid fuel; biomass pyrolysis for high-value products. She has published more than 60 papers. She was an excellent youth winner of Natural Science Foundation Project. Published articles from *Fuel* (2007, 86: 1781-1788) and *Energy & Fuels* (2006, 20(1):388-393) have been cited in ESI database from 2010. So far the number of citation in web of science for the two papers is 1367 and 313, respectively. The paper in *Fuel* journal is also one of the most downloaded and cited one.

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Raquel Viveiros et al., Trends in Green chem, 3:2
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Green design of lock-and-key affinity devices to address API purification challenges

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[2]Hovione FarmaCiencia, Portugal

Statement of the Problem: Pharmaceutical industry spends a very significant amount of its financial resources in API (Active Pharmaceutic Ingredients) purification processes to comply with impurity limits imposed by regulatory agencies (FDA and EMEA). To address this worldwide demand, several purification materials have been proposed, such as molecular imprinted polymers (MIPs). These lock-and-key affinity materials can be produced by different conventional approaches. In the last years, the use of the Green Chemistry principles has changed the way polymers can be produced. Green technologies applied to MIP development are appearing not only due the environment issues but also by the features of the final product and cost-effective production from the point of view of industry. MIPs have been developed in our lab using supercritical carbon dioxide ($scCO_2$) technology. These affinity materials have been obtained for wide range of applications, namely pharmaceutical impurity removal, enrichment of natural products, removal of contaminants from diesel and from water ressources. Lock-and-key affinity materials are obtained as ready-to-use and easy-to-handle dry-powders of homogenous particle sizes, without organic solvent residues.

Methodology & Theoretical Orientation: With the aim of achieving lock-and-key affinity materials to address efficiently API pharma demand, several strategies were explored using $scCO_2$ (Figure 1). Herein we show three case studies, including (i) the synthesis of high affinity polymers for API impurity; (ii) the production of large core-shell affinity beads for gravity-driven purification processes and (iii) the use of computational tools to perform the rational design and optimization of the affinity materials, in which the CO_2 was introduced for the first time as the solvent in the molecular modelling simulations, for a cheaper and less time-consuming processes.

Conclusion & Significance: The affinity materials produced in $scCO_2$ are obtained in a green way, bringing advantages to the process itself such as by reducing the use of organic solvents, and mechanical crushing and sieving compared to conventional processes, as well as to advantages over other affinity molecules such as antibodies and enzymes: they are stable over harsh pH, pH and temperature conditions, they are reusable and robust, whilst obtained in high purity and ready-to-use. In addition, results obtained in the 3 examples mentioned above revealed a good performance in API impurity removal. We also show that computational approaches are an added-value tool and key advantage in the rational design of the best affinity systems when using a green technology, avoiding hard and time-consuming screening methodologies and consequently reducing time and organic solvents consumption.

Figure 1: Different approaches on lock-and-key affinity devices for API purification.

Biography

Raquel Viveiros is finishing her PhD project in Sustainable Chemistry in collaboration between NOVA University of Lisbon and a pharmaceutical company Hovione. She performed a short training ship at the Prof. Sergey Pilestky´s Biotechnology group at University of Leicester on solid-phase synthesis and molecular modeling systems. She also worked as Research Fellow in the several projects related to the development of affinity devices for different applications. Her multidisciplinary professional background covers green chemistry, organic and analytical chemistry, molecular recognition, molecular imprinting, process development, and pharmaceutical purification processes. In addition, last year she was team member of COHiTEC 2016, a training program in technology commercialization.

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Almudena Lorente et al., Trends in Green chem, 3:2
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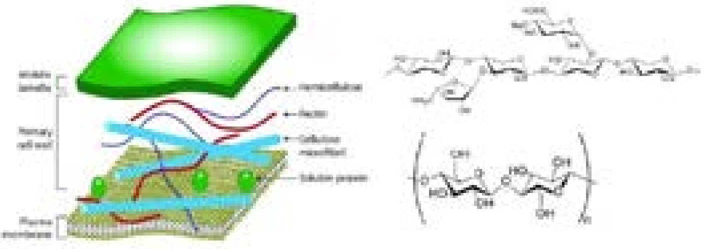
Valorization of lignocellulosic biomass and production of biofuel precursors under microwave radiation

Almudena Lorente*, **Covadonga Lucas-Torres**, **Maria Prado Sanchez-Verdu** and **Andres Moreno**
University of Castilla La Mancha (UCLM), Spain

Fossil fuel reserves are nowadays decreasing and their use cause high CO_2 emissions. For these reasons lignocellulosic biomass is becoming increasingly recognised as a good feedstock and carbon source with different components and applications. Microwave radiation is a green energy technique for the hydrolysis and dehydration of biomass into monosaccharides due to the reduction of reaction times and the elimination of reaction by-products. Plant cell wall is mainly composed by cellulose, hemicellulose and lignin. Cellulose is the predominant component which can be hydrolyzed into glucose and then dehydrated under microwave radiation in acidic medium and at high temperature to obtain 5-hydroxymethylfurfural (HMF) and levulinic acid (LA), both of them well-known biofuel precursors. Hence, the aim of this work is the study of the hydrolysis and dehydration of microcrystalline cellulose by microwave radiation using homogeneous and heterogeneous catalysts and different reaction systems. The optimal conditions obtained have been applied for the obtaining of HMF and LA from some waste such as beer bagasse and melon rind. For conclusion, this work has been able to obtain biofuel precursors from waste using a green and environmentally friendly energy such as microwave radiation, also we have developed different methods to obtain one precursor or another using different pretreatment and changing experimental conditions.



Biography

Almudena Lorente Diezma was born on February 1991 in Toledo (Spain). She obtained her degree in Chemistry in June 2014 at the University of Castilla La Mancha. Her first contact with Organic Chemistry and Microwave assisted was in her fifth year of degree in the group ´Organic Green Chemistry. Food and agroindustrial waste Chemistry`. Then on November 2014 she started her PhD in the same group with the Thesis title ´Obtención de nuevos biocombustibles de 2ª generación y sus implicaciones atmosféricas`. During these years she has continued her training in the field of waste and Bioeconomy. She obtained her certificate about Bioeconomy studies in September 2016.

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Notes:

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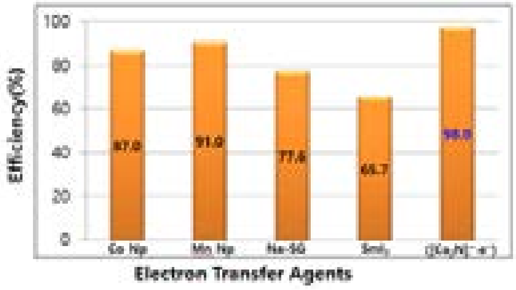
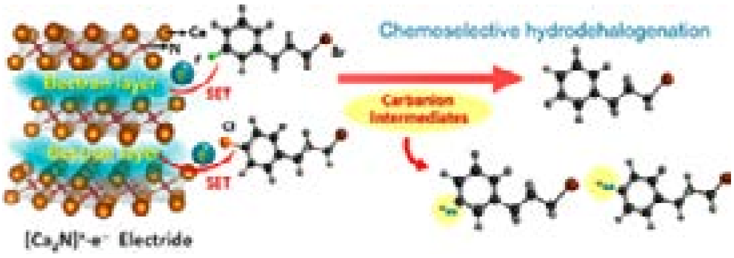
Chemoselective hydrodehalogenation and high efficiency birch reduction using two-dimensional inorganic electride dicalcium nitride ([Ca$_2$n] +·e-) as a reducing agent

Byung Il You, Ye Ji Kim and **Sung Wng Kim**
Sungkyunkwan University, Republic of Korea

Polycyclic aromatic and halogenated organic compounds are known as a functional material which has applications in chemical industry, biology, pharmacology. Inspite of the utility of polycyclic aromatic and halogenated hydrocarbons, it has concerns about human health such as carcinogenic or mutagenic risk and considerable environmental pollution. In hydrogenation of polycyclic aromatic hydrocarbons (Birch reduction) and dehalogenation reactions, the consecutive single-electron transfer from reducing agents generates the radical and corresponding carbanion and removes the halogen atom and π–conjugated electron in polycyclic aromatic compounds. The most prominent feature of two-dimensional electride [Ca$_2$N] +·e$^-$- is powerful electron donating nature as reductant originated from high electron concentration and low work-function. The electron donating ability of two-dimensional electride was demonstrated through single electron transfer involving chemical reactions such as pinacol coupling reaction, trifluoromethylation, transfer hydrogenation. Herein, we report a new strategy for efficient chemoselective hydrodehalogenation through the formation of stable carbanion intermediates, which are simply and birch reduction of polycyclic aromatic rings by using the anionic electrons of two dimensional inorganic electride [Ca$_2$N]+·e$^-$-with effective electron transfer ability. The consecutive single-electron transfer from inorganic electride [Ca$_2$N] +·e$^-$- stabilized free cabanions, which is a key step in achieving the selective reaction. The control of equivalent of inorganic electride [Ca$_2$N] +·e$^-$-and reaction condition provided exceptional reactivity in comparison with other reducing agents such as cobalt nanoparticle, manganese nanoparticle, Samarium iodide (SmI$_2$) and sodium silica-gel. Also, a determinant more important than leaving group ability is the stability control of free carbanions according to the s character determined by the backbone structure. We anticipate that this approach may provide new insight into selective chemical formation, including hydrodehalogenation.





Biography

Byung Il Yoo got his Bachelor’s degree in Department of Chemistry from Korea Advanced Institute of Science and Technology in 2014. Since 2016, he joined prof. Sung Wng Kim’s group of Sungkyunkwan University as Post-Graduate student. He research interest includes synthesis new type of inorganic electride, chemical application of inorganic electride.

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Notes:

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The new class of green material: Two-dimensional electride [Ca$_2$N]+·e-

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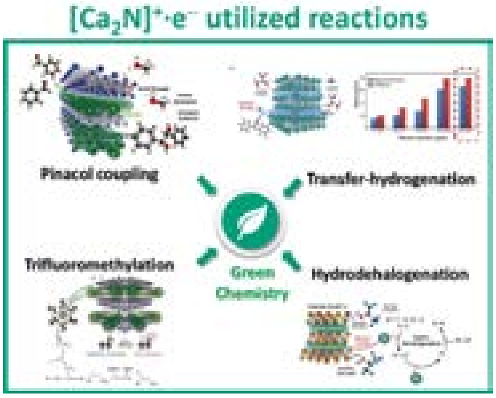
Electrides, which are ionic crystals trapping anionic electrons in the structural cavities, have attracted attention due to their exotic properties such as a low work function. The first crystalline organic electride was synthesized from solvated electron, alkali metal-ammonia solutions, by James L. Dye in 1983. The temperature instability of organic electride have been solved by the discovery of room temperature stable inorganic electrides [Ca$_{24}$Al$_{28}$O$_{64}$]4+·4e-)] and [Ca$_2$N]+·e-. The [Ca$_2$N]+·e- electride showed the delocalized anionic electrons within the interlayer spacing of ~0.4 nm, showing the low work function value of 2.6 eV with the electron concentration of~1.37 x1022 cm^{-3}, which are comparable to typical alkali metals. Due to low work function and high electron concentration, an outstanding performance in organic chemical synthesis such as with high electron transfer ability has been anticipated. Charge transfer in and out of inorganic/organic materials from and to counterpart materials is a key issue to promote the chemical reactions. In the organic chemistry, there are important intermediates that are generated by charged transfer; carbanion or radical. To produce the radical or carbanion intermediates, single electron transfer agents or photo catalysts such as samarium iodide, iridium complex and cadmium alloys was generally utilized. However, the usage of transition metals and rare-earth metals which has the toxicity for human bodies and environmentally harmful residual products. In view of sustainable green chemistry, the electride which consisted of earth abundant elements (calcium and nitrogen) utilized reaction system could be the promising solution. In this talk, several inorganic electride utilized organic reactions, pinacol coupling reactions, trifluoromethylations, transfer-hydrogenations and hydrodehalogenations, will be introduced as a new strategy for organic synthetic chemistry.



Biography

Ye Ji Kim got her Bachelor's degree in Chemistry from Kyungsung University in 2013. Since 2013, she joined prof. Sung Wng Kim's group of Sungkyunkwan University as post-graduate student. Her research interest include chemical application of inorganic electride, single electron transfer reaction, hydrogen evolution reaction and nano-particle fabrication. Prof. Sung Wng Kim's group's research interests mainly focus on the development of inorganic electrides and its chemical and physical applications, thermoelectrics and transition metal dichalcogenide. Prof. Sung Wng Kim has published about 100 SCI papers in leading of journals of natural science, such as Science, Nature , Nature serious journals, JACS, Adv. Mater., Nano letters.

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Isreal Ugochukwu Oshiojum et al., Trends in Green chem, 3:2
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Phytoremediation of heavy metal-polluted aquatic ecosystem (Ologe Lagoon) by water hyacinth (*Eichhornia crassipes* [mart.] solms) and the socio-ecological implications

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[1]Lagos State University, Nigeria
[2]University of Ibadan, Nigeria
[3]Lagos State University, Nigeria

The indiscriminate discharge of industrial effluents containing harmful substances such as heavy metals has become a global problem because of the negative effects of these substances on humans. Water hyacinth (*Eichhornia crassipes*) has been considered a menace since it entered Nigerian inland waters through neighbouring Republic of Benin in the 80's. Attempts to eradicate it has not been successful. Thus, there is a need to explore its useful potentials. It is used in paper production, feed formulation, phytoremediation, etc. Phytoremediation is a bioremediation process that uses plants to remove, transfer, stabilize, and/or destroy pollutants in the soil and water. This study investigated the ability of water hyacinth in passive phytoremediation of heavy-metal polluted aquatic ecosystems and the socio-ecological effects of the plant's invasiveness. The study was conducted over a period of 18 months (July, 2013 – December, 2014) and 5 sampling stations (Owo River, Agbara, Otto Jetty, Morogbo and Etegbin) were chosen based on proximity to points of discharge of effluents, presence of water hyacinth and human activities. The metals investigated are Cu, Zn, Pb, Fe, Cd and As. The result showed that water hyacinth absorbs heavy metals from its environment and the rate of absorption depends on concentration of the metal. It was also discovered that the presence of water hyacinth and illegal sand-mining has adversely affected the delivery of ecosystem services such as fisheries, tourism, etc. The consequences of these unregulated anthropogenic actions cause loss in biodiversity, food insecurity and ultimately threat human lives.

Biography

Isreal Ugochukwu Oshiojum is currently working in Department of Fisheries at Lagos State University, Nigeria. He is an expert with specialization in Aquaculture and Ecology.

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Notes:

Bingxin Yuan et al., Trends in Green chem, 3:2
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Reusable cobalt-phthalocyanine in water: Efficient catalytic aerobic oxidative coupling of thiols to synthesize organosulfur compounds

Bingxin Yuan, Xin Huang, Liting Yang, Yingchao Dou, Shan Zhen, Lijuan Song, Heng Li, Panke Zhang and **Guanyu Yang**
Zhengzhou University, China

Statement of the Problem: Organosulfur compounds have been vitally applied as synthetic intermediates and reagents in organic synthesis, pharmaceutical and biological science. Nevertheless, the shortcomings of traditional methods are apparent, including toxic organic waste, harsh reaction conditions (such as high temperature, long reaction hours, and risk of over-oxidation), extra additives or bases, and tedious work-up procedures. Therefore, the development of novel and green strategies that can be carried out under mild conditions for the synthesis of organosulfur compounds remains a challenge and is highly desired. In this contribution, we describe the catalytic aerobic oxidation of thiols to synthesize disulfides, sulfonamides and diaryl sulfides. A reusable cobalt-e catalyzed aerobic oxidative coupling of thiols to produce disulfides and sulfonamides in water was studied, which utilizes environmentally friendly and naturally abundant O_2 as the oxidant.

Findings: The mother liquor could be recycled up to 20 times with negligible loss of activity and only a minor decrease of product yield. The same catalytic system was further extended to oxidative cross-coupling of naphthol/naphthylamine with thiols to form diaryl sulfides bearing a wide range of substituents in good to excellent yields.

Conclusion & Significance: These highly efficient and versatile methodologies offer interesting prospects for the commercial manufacturing of organosulfur compounds in a much greener and economical way.

Biography

Bingxin Yuan, PhD is an Assistant Professor of College of Chemistry and Molecular Engineering in Zhegnzhou University since 2016. She pursued her PhD degree in organic Chemistry in USA and graduated in Aug, 2016. She started working in Zhengzhou University ever since. She has her expertise in novel organic synthesis and organic semiconducting materials synthesis and characterization. Her work aim to address the challenges of organic synthesis in a greener way: design and study of green catalysis with unique chemical properties. Her main research fields contain the radical and oxidative reaction as novel synthetic tools that are non-hazardous and environmentally friendly for manufacture of chemicals.

Guanyu Yang is a Professor in College of Chemistry and Molecular Engineering, Zhengzhou University, China, since 2006. He received his Ph.D. of chemistry in 2005 from Dalian Institute of Physical Chemistry, Chinese Academy of Sciences. His research interests center around the development of new synthetic methodologies, and the more environmentally benign processes for the synthesis of higher added-value chemicals. For this aim, his research directs towards the fundamental and applicable investigations of various catalytic techniques, involving organo-, biomimetic, heterogenous, and homogenous catalysis, as well as the interdisciplinary approach. Much of his work is devoted to the development of novel synthetic methods via the catalytic oxidation with molecular oxygen as a terminal oxidant.

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