

11th Edition of
International Conference on

CATALYSIS,
CHEMICAL
ENGINEERING
AND
TECHNOLOGY

16-17

MAY 2022

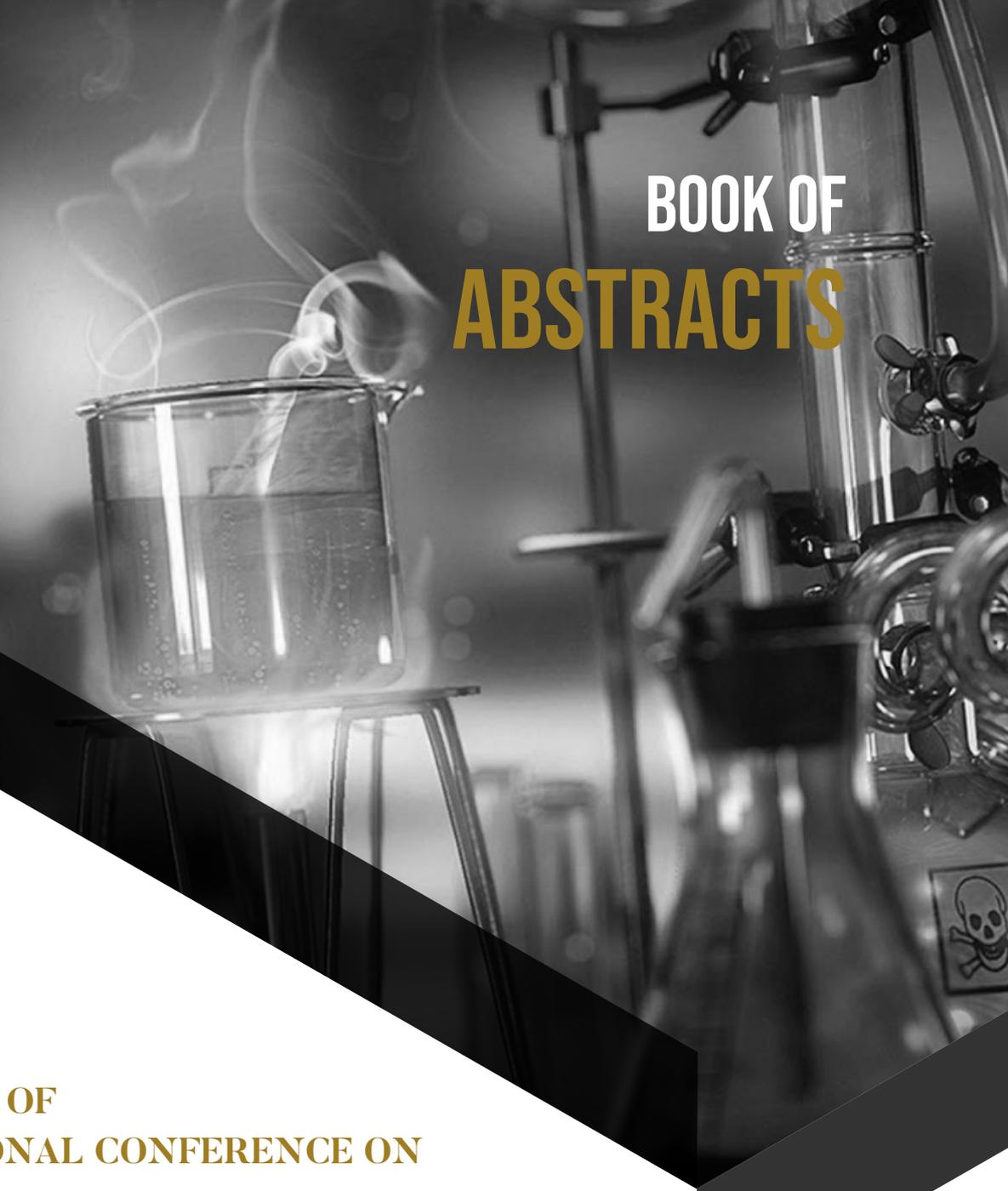
VIRTUAL EVENT

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Ph: +1 (702) 988-2320

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Website: <https://catalysis-conferences.com/>



**BOOK OF
ABSTRACTS**

**11TH EDITION OF
INTERNATIONAL CONFERENCE ON
CATALYSIS, CHEMICAL
ENGINEERING AND
TECHNOLOGY**

16-17 **MAY**

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ABOUT MAGNUS GROUP

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

Participation from 90 different countries and 1090 different Universities have contributed to the success of our conferences. Our first International Conference was organized on Oncology and Radiology (ICOR) in Dubai, UAE. Our conferences usually run for 2-3 days completely covering Keynote & Oral sessions along with workshops and poster presentations. Our organization runs promptly with dedicated and proficient employees’ managing different conferences throughout the world, without compromising service and quality.



ABOUT CCT 2022

CCT 2022 welcomes members from different parts of the world to join our Online Event - “11th Edition of International Conference on Catalysis, Chemical Engineering and Technology” scheduled during May 16-17, 2022. It includes prompt Keynote presentations, Oral presentations, and Poster presentations, interactive and informal exchanges. This is going to be one of the most remarkable events of the year. Through the theme “Exploring critical breakthroughs in Catalysis and chemical engineering” conference will explore the advances in the field. CCT 2022 goal is to bring together bright minds to give talks that are ideas-focused, and on a wide range of scientific sessions, to faster learning inspiration. It will provide an international platform to share expertise, foster collaborations, discover new information, and stay current with trends and networking.



KEYNOTE FORUM

DAY 01

11TH EDITION OF
INTERNATIONAL CONFERENCE ON
**CATALYSIS, CHEMICAL
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TECHNOLOGY**

16-17 MAY



Thomas J. J. Müller

Heinrich-Heine-Universität Dusseldorf, Germany

With one catalyst in multiple steps in one-pot fashion-sequentially palladium-catalyzed processes for the synthesis of functional heterocycles

One-pot reactions, if conducted in a consecutive, sequential or domino fashion, promise a highly efficient and efficacious synthetic access to many functional molecules of interest. In particular, heterocyclic systems are interesting due to their vast spectrum of applications. Transition metal catalyzed multi-component sequences have recently gained a considerable interest since they enable transformations with high tolerance of functional groups. Over the years we have established Pd-catalyzed entries to ynones, diynones, diynes, enals, enones, and boronates, which are valuable intermediates for in situ transformation into complex molecules in a one-pot fashion. Likewise, sequentially Pd-catalyzed processes have opened new avenues to one-pot syntheses of numerous classes of heterocyclic frameworks. Most interestingly, in sequentially Pd-catalyzed processes the same catalyst source is operative a second time without further catalyst addition. This one-pot methodological concept is most elegantly applied to the syntheses of various classes of functional heterocycles, ranging from functional chromophores and electrophores to luminophore, and as a key step in very concise syntheses of marine alkaloids, kinase inhibitors and anti-infectiva. By virtue, concise accesses to substance libraries of interest in organic materials and life sciences are efficiently enabled.

Audience Take Away:

- Multicomponent reactions allow for assembling relatively complex structures in a concise and efficient way.
- Substance libraries are readily obtained with avoiding multi-step and multi-work up operations.
- Enhanced lead finding can be done in a one-process more efficaciously and this is always superior to multi-operation sequences.
- The conceptual approach is a reactivity-based concatenation of quite various reactivity of the underlying functionalities in a single reaction vessel to allow for a concise sequence.
- The combination of catalytic and even catalyst economic one-pot methodologies with targeting functional molecules of interest (chromophores, electrophores, fluorophores, pharmacophores) provides novel structures but simultaneously represents a greener approach to efficient chemistry, which is definitively in the focus at times of climate change and shrinking resources.

Biography

Thomas J. J. Müller studied chemistry (1984-1989) at the University of München (LMU) (diploma 1989; Ph.D. 1992). After a post-doctoral stay at Stanford University (1993/1994), he developed his independent research at Technical University Darmstadt and LMU (1994-1999; habilitation 2000). After a professorship at the University of Heidelberg (2002-2006) he is a chaired full professor at the University of Düsseldorf since 2006, and since 2019 the spokesman of the Research Training Group 2482 funded by the German Science Foundation (DFG). His research interests encompass synthetic and physical-organic chemistry of functional chromophores, and the design of novel one-pot reactions, documented in more than 300 publications.



V. Beschkov*, L. Ljutzkanov, E. Razkazova-Velkova, N. Dermenjieva, S. Stefanov

Bulgarian Academy of Sciences, Bulgaria

On the catalytic conversions of sulfide ions in sulfide-driven fuel cells

Hydrogen sulfide is met in different natural sources, like the deep waters of the Black Sea, some closed water ponds, natural springs of mineral water, etc. It is also present in some effluents at oil processing by de-sulfurization. A straightforward method to remove hydrogen sulfide is to convert it into sulfate in sulfide-driven fuel cells (SDFC). This process is accompanied by generation of energy directly as electricity.

A problem of this application is the big variety of sulfur compounds of different valences leading to incomplete sulfide conversion and lower energy yield. This problem must be overcome by the use of selective catalysts able to promote the complete conversion of sulfide to sulfate.

The present work comprises the results of the use of different compounds of metal ions, namely zirconia, cobalt spinel, zinc oxide. The study on their catalytic activity shows the advantages of zinc oxide embedded in pyrolysed carbon source for the complete conversion of sulfide to sulfate. Lab-scale experiments show that the fuel cell application is a direct method for hydrogen sulfide removal either for environmental or energy benefits.

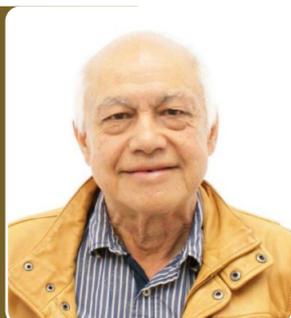
This work was supported by the program Eplus, Ministry of Education and Science, Republic of Bulgaria

Audience Take Away:

- Knowledge about fuel cells. Catalytic properties of heavy metals for sulfide oxidation
- The combination of environmental issue and energy production could be applied elsewhere.

Biography

Venko Beschkov, PhD was born in 1946 in Sofia, Bulgaria. He has got his PhD in 1978 and his DSc degree in 1996 in the Bulgarian Academy of Sciences. His present interests are chemical and biochemical processes for environment protection and for utilization of renewable energy sources. He participates in 30 scientific projects and in 18 applied ones. He published over 210 scientific papers, 2 monographs and 10 chapters in selected issues. He has been Head of the Institute of Chemical Engineering at the Bulgarian Academy of Sciences for 21 years (1993/2014) and deputy-minister of environment (1991/92).

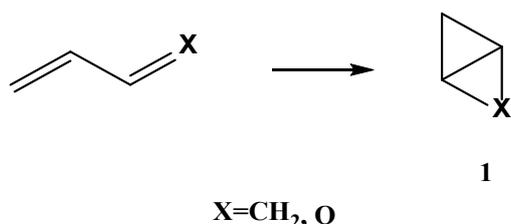


Anita Ragyanszki, Bela Fiser, Edward Lee-Ruff *,
Joel F. Liebman

York University, Canada

Photochemical valence isomerization to high energy products- bicyclobutanes and oxabicyclobutanes

The photochemical valence isomerization of 1,3-butadienes give bicyclobutane 1($X=CH_2$). The stereochemistry of these strained products in substituted derivatives suggest a double disrotatory ring cyclization originating from the second excited state of the diene. The oxygen analog valence isomerization from acrolein has not been reported nor its product, oxabicyclobutane 1($X=O$). DFT computations for both bicyclics showed a large basicity for the carbon analog exceeding that of the oxygen analog. The strain energy for oxabicyclobutane exceeds that for bicyclobutane. The validity of the computational method is seen from the congruence between experimental and computational values of the structural and thermochemical parameters



Audience Take Away:

- Audience will learn about principles of photochemistry.
- Introduction of strain and determination of strain energy
- Definition of proton affinity and basicity.
- Illustration of valence isomerizations.

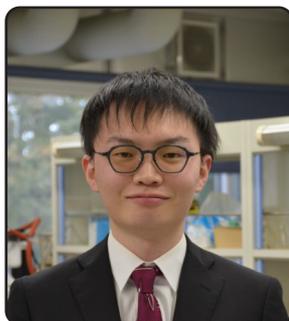
Biography

He obtained his B.Sc. and Ph.D. from McGill University. He spent his postdoctoral studies at Columbia University, New York. He is currently Emeritus Professor after 45 years at York University. He has over 140 publications in peer reviewed journals and was awarded the Fellowship of the Canadian Institute of Chemistry. He has had 41 years of continuous government research support. His research also lead to two patents. He is also consultant for patent attorneys in litigation cases between generic and brand name drug companies. He has been involved in the outreach program giving lectures on patent issues between generic and brand name drugs.

POSTERS
DAY 01

**11TH EDITION OF
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16-17 **MAY**



Yuto Nakano*, Keita Kashima, Masanao Imai, Peter Walde

National Institute of Technology, Oyama College, Japan

How industrial laccase and anionic vesicles work on an oxidation of the miscible substrates consisting of aniline and *p*-aminodiphenylamine in order to synthesize polyaniline in its conductive emeraldine salt form

Industrial laccase-catalyzed oxidation of the miscible substrates consisting of aniline and *p*-aminodiphenylamine (PADPA) in the presence of vesicles from sodium bis (2-ethylhexyl) sulfosuccinate (AOT) as templates was multilaterally investigated. Reaction products with their kinetic development were analyzed with in situ ultraviolet/visible/near infrared spectroscopy (UV/Vis/NIR), in situ electron paramagnetic resonance (EPR), and ex situ liquid chromatography with photodiode array detector/mass spectrometry (LC-PDA/MS). In addition, the oxidizing activity of industrial laccase was evaluated by 2,2'-azino-bis (3-ethylbenzothiazoline-6-sulfonic acid) diammonium salt (ABTS).

The reaction condition was preliminarily optimized based on in situ UV/Vis/NIR measurement. The reaction mixture obtained from [aniline] + [PADPA] = 0.6 mM + 0.7 mM, [AOT vesicles] = 1.5 mM, [laccase Y120] = 17 nM colored to dark green, and notably developed absorption peaks at $\lambda \approx 420, 1000$ nm corresponding to formation of polaron (radical cations) until 24 h. In situ EPR measurement revealed that the reaction products contained significant radicals, which confirms polyaniline in its conductive emeraldine salt form (PANI-ES)-like products obtained. For ex situ LC-PDA/MS measurements of the extracted, deprotonated, and reduced products after 1 week, the main products were aniline tetramer while aniline and PADPA were almost consumed.

In contrast, the reaction products without AOT vesicles only colored to reddish-purple with small peak at $\lambda \approx 800$ nm and no signal was observed in EPR. The reaction without laccase remained colorless and polaron was not detected UV/Vis/NIR and EPR. The comparative evaluation indicates both laccase and vesicles lead to the selective synthesis of PANI-ES.

Since the kinetic evaluation of the oxidizing activity of industrial laccase on ABTS, the presence of AOT vesicles decreased the maximum reaction rate V_{max} , the turnover number (k_{cat}) and Michaelis coefficient K_m , however increased Hill coefficient n slightly. It was predicted that the protonated substrates in the acidic solution were loosely constrained on anionic interface of AOT vesicles. Therefore, the compatibility between substrates and laccase was advanced apparently.

The oxidation of aniline and PADPA was carried out at room temperature ($T \approx 25^\circ\text{C}$) in a phosphate solution of pH = 3.5 (0.1 M $\text{NaH}_2\text{PO}_4 + \text{H}_3\text{PO}_4$). This process is environmentally friendlier than the traditional chemical synthesis of PANI-ES, which occurs at strongly acidic conditions and a strong chemical oxidant, such as potassium dichromate or ammonium peroxodisulfate. Industrial laccase-catalyzed synthesis of PANI-ES in the presence of AOT vesicles as templates is promising to green chemical engineering environmentally as well as economically.

Audience Take Away:

- Green chemical synthesis of electro-conductive polyaniline
- Details of characterization for enzymatic oxidation of aniline and its dimer PADPA
- Information of soft interfaces, especially vesicles, guiding the oxidative reaction
- Utilization of industrial laccase as an oxidant for material production

Biography

Mr. Yuto Nakano have studied chemical engineering, organic chemistry, inorganic chemistry, physical chemistry, and bioengineering at Department of Materials Chemistry and Bioengineering in National Institute of Technology, Oyama College (Oyama KOSEN) since 2016 for 5years. Afterward, he proceeded the advanced course of National Institute of Technology, Oyama College 2021. Mr. Nakano currently works on the enzymatic synthesis of conductive polyaniline in Laboratory of Chemical Engineering



Yakha Vissurkhanova*, N. M. Ivanova, E. A. Soboleva

E. A. Buketov Karaganda University, Kazakhstan

Fabrication of Fe-Cu catalysts on the basis of copper (II) ferrite

This paper describes the results of the investigation on the ability of copper(II) ferrite (CuFe_2O_4) to reduction in an electrochemical system with the formation of Fe-Cu composites. The effect of a polymer stabilizer (polyvinyl alcohol, PVA) on structural and phase changes in CuFe_2O_4 during thermal treatment and subsequent electrochemical reduction has been studied. The electrocatalytic properties of Fe-Cu composites have been tested in reactions of electrohydrogenation of *p*-nitrobenzoic acid (*p*-NBA) and acetophenone (APh).

Copper(II) ferrite was synthesized by co-precipitation method from aqueous solutions of copper(II) nitrate and ferric(III) chloride (1:2 molar ratio) without and with the addition of polymer via NaOH. The resulting precipitate was filtered and washed with distilled water. Dried CuFe_2O_4 and CuFe_2O_4 +PVA samples were thermally treated at 500°C, 700°C and 900°C for 2 hours.

According to XRD results, the copper ferrite samples thermally treated at three temperatures have CuFe_2O_4 crystalline phases with corresponding peaks of high intensity and CuO in a small amount. The electrochemical reduction of these samples is accompanied by the formation of phase constitutions that differ significantly from each other. Thus, in the CuFe_2O_4 (500°C) sample copper cations are reduced in a larger amount than iron cations, magnetite is formed (with a possible residue of CuFe_2O_4), and Cu_2O crystalline phases appear. In the composition of CuFe_2O_4 (700°C) sample the ratio of reduced metals is approximately equal with a slight predominance of iron and a sharp decrease in the Fe_3O_4 content. In the CuFe_2O_4 (900°C) sample, the amount of electrochemically reduced iron becomes significantly higher than that of copper. It is concluded that the temperature of heat treatment affects the phase constitution of Fe-Cu composites during reduction in the electrochemical system and the relative content of both metals.

Co-precipitation of CuFe_2O_4 precursors from an aqueous solution of PVA and subsequent thermal treatment of prepared CuFe_2O_4 samples lead to the formation of composites whose phase constitutions differ from those prepared without a polymer. In all thermally treated CuFe_2O_4 +PVA samples in addition to CuFe_2O_4 crystalline phases, the reduced metals appear: Cu^0 (500°C), $\text{Fe}^0 > \text{Cu}^0$ (700°C) and $\text{Fe}^0 \leq \text{Cu}^0$ (900°C), which are obviously formed under the action of polymer decomposition products. In the electrochemical system, additional reduction of metal cations occurs in thermally treated CuFe_2O_4 +PVA samples. The amount of reduced metals increases, and compared to the samples synthesized without polymer, their relative content changes: $\text{Fe}^0 < \text{Cu}^0$ (500°C), $\text{Fe}^0 \leq \text{Cu}^0$ (700°C) and $\text{Fe}^0 = \text{Cu}^0$ (900°C).

The Fe-Cu composites obtained after thermal treatment and electrochemical reduction were used as electrocatalysts in the electrohydrogenation of *p*-NBA and APh. The experiments were carried out in a diaphragm cell on a copper cathode in the aqueous-alcoholic-alkaline catholyte at a current of 1.5 A and temperature of 30°C, the anode was a Pt-grid. It was established that the all Fe-Cu composites have electrocatalytic activity, increasing the hydrogenation rate and conversion of *p*-NBA and APh in comparison with their electrochemical reduction on a Cu cathode (without catalyst). Fe-Cu catalysts prepared in this way can be used in various catalytic and electrocatalytic processes.

Biography

Yakha Vissurkhanova is a 3rd year PhD student of Academician E. A. Buketov Karaganda University. Since 2012 she has been working as Researcher at Institute of Organic Synthesis and Chemistry of Coal of Kazakhstan Republic. Her research activities are focused on the synthesis of metal-polymer composites, metal ferrites, metal-carbon composites and the investigation of their electrocatalytic activity in electrosynthesis of organic compounds. She has published more than 17 research papers in various reputed national and international journals.



Anna M. Kisiela-Czajka

Wroclaw University of Science and Technology, Poland

Chemico-instrumental methods of functional groups analysis

The thermal conversion of fossil solid fuels, car tires, biomass, or sewage sludge leads to significant amounts of waste, for which developing a direction for safe disposal can be a complex issue. This group is characterized above all by a high concentration of carbon in its chemical composition and, depending on its origin, by the presence of oxygen, hydrogen, and nitrogen heteroatoms, which, being part of surface complexes, may constitute active sites capable of forming bonds with the reactant molecule in a given chemical reaction. The groups that determine the practical utility of the carbon materials are those consisting of carbon and/or hydrogen atom bonded to an oxygen atom. These groups determine the adsorption, catalytic, oxidation-reducing, and acid-base properties, which are key e.g. for adsorption-catalytic gas purification.

Despite extensive work, the nature of surface functional groups has not been fully elucidated. Difficulties in interpreting the obtained test results are mainly due to the complexity of the structure of the carbon substance. The range of techniques available is also debatable. Moreover, the surface carbon-oxygen groups, formed as a result of the interaction of the carbon material with the oxidant, are characterized by different thermal stability. Consequently, under inert atmosphere conditions and at high temperatures, their conversion to specific gaseous products occurs. As carbon materials have high reactivity with oxygen, these groups are typically released into carbon monoxide and dioxide, and water vapor. The thermal stability of the functional groups is very important because many of the high carbonaceous waste management directions require thermal treatment. Although the mechanism of thermal decomposition of functional groups is well understood, the kinetics is already difficult to reveal due to the overlap of intermediate reactions. Considering the above, to complement the characterization of surface groups obtained by titration techniques, infrared spectroscopic analysis in KBr and Raman modes was carried out. The use of different types of electromagnetic radiation gave the possibility to observe in the spectra bands characteristic for particular functional groups (with single and multiple bonds between atoms). The proposed procedure, thanks to the complementarity of the techniques, enabled to significantly extend the range of obtained information on the surface functional groups. The subjects of the research were high carbonaceous waste of the combustion process, i.e.: selected fractions of unburned carbon from lignite and coal fly ash, petroleum coke, char formed by pyrolysis of MDF boards, and zeolite - as precursors of carbon adsorbents/catalysts in the process of removal/reduction of NO_x , SO_2 , NH_3 , CO_2 and commercial activated carbons from coal dust, dedicated to the purification of flue gases precisely. In addition, an attempt was made to describe the chemical kinetics of the decomposition of functional groups by TGA, with identification of gaseous products by FTIR and analysis of the thermal character of the separated products by DSC. A one-step model was used to separate the steps of the different individuals, taking into account the mechanism of multiple parallel reactions. The desorption rate of the oxide layer was described by the Arrhenius equation.

Audience Take Away:

- Complementing the titration analysis with an instrumental analysis provides a reliable picture of the chemical structure;
- The use of various types of electromagnetic radiation makes it possible to observe in the spectra the bands characteristic of particular functional groups (with single and multiple bonds between atoms);
- The thermal stability of the functional groups is very important, as many of the management directions of high carbonaceous waste require thermal treatment or are carried out at a temperature higher than 150 °C (for which the decomposition of functional groups is observed).

Biography

Graduate of the Faculty of Chemistry and Mechanical and Power Engineering, doctor of Technical Sciences in Power Engineering since 2018, and currently an assistant professor in the Department of Energy Conversion Engineering at Wrocław University of Science and Technology. Interested in: synthesis of adsorbents/catalysts from high carbonaceous waste, functionalization of the porous structure, titration analysis and spectroscopy in the study of surface functional groups, modeling chemical kinetics with elements of statistics, flue gases treatment/process gases storage and process equipment. Currently involved in Polish-South African cooperation in the field of reducing nitrogen oxides by heterogeneous catalysis, under conditions of a low technical minimum power boiler.

**Demirov A.P.*, Sergevinin V.S., Chernogor A.V, Belov D.S. and Blinkov I.V.**

National University of Science and Technology MISIS, Russian Federation

Photocatalytic behavior of films based on hollow hematite microspheres

Hematite ($\alpha\text{-Fe}_2\text{O}_3$) is a promising material for photoanode. However, it has a few drawbacks as low concentration of charge carriers and low OER kinetic. These disadvantages fix by morphology control and doping.

The study is dedicated to the photoelectrochemical behavior of films based on $\alpha\text{-Fe}_2\text{O}_3$ hollow submicron spheres. Spheres with an average size of 970 nm and wall thickness of about 300 nm were received by the spray-pyrolysis method. The structure of the synthesized particles implies the presence of pores inside the particles. Well-known that the concentration of vacancies near the pore is more than equilibrium. Also, oxygen vacancies in $\alpha\text{-Fe}_2\text{O}_3$ are donor dopants. Therefore, the bottom of the conduction band near the interface wall/pore is lower than at the interface wall/electrolyte. This structure provides a higher charge separation.

Films were produced by Dr. Blade method. FTO-glass was used as a substrate, a mixture of 20 % (wt.) aqueous solution of $\text{Fe}(\text{NO}_3)_3$ and hollow submicron sphere $\alpha\text{-Fe}_2\text{O}_3$ in ratio 2 : 3 was used as slurry. Samples were annealed at 400 °C for 1 hour with heating rate 2 °C/min at air. Morphology and phase composition of samples were obtained by scanning electron microscopy (SEM) (Vega 3 Tescan, Czech Republic) and X-ray diffraction (XRD) (Difrey-401, Russia). At the cross-section SEM-image was seen two-level structure consisting of nanoparticles layer and submicron particles layer with film thickness 5 μm . At the surface was found “necks” between submicron particles. Nanoparticles layer and “necks” were formed as result $\text{Fe}(\text{NO}_3)_3$ decomposition. XRD analysis was shown that only hematite phase in the film.

Photoelectrochemical behavior of the film was studied in 0.1M KOH aqueous solution using hand-made three electrode photoelectrochemical cell (SCE electrode was used as reference, graphite electrode was auxiliary, sample was work electrode), potentiostat P-45X (Electrochemical Instruments, Russia) and Xenon solar light source (Newport, USA) (solar illumination 100 mW/cm²). Contact area between the sample and electrolyte and illuminated area was 1 cm². Photovoltage was determined as difference of open circuit potential in dark and under illumination (VOC). Current-voltage (J-V) in the dark, stationary current-time curves (J-t) with chopped illumination were recorded. VOC of the sample was 150 mV. J-V plots in the dark shown that onset potential is about 0.87 V vs SCE (1, 13 V vs RHE). J-t plots recorded at 0 – 0.8 V vs SCE with chopped illumination shown that photocurrent density was stable and equal 1 – 4 $\mu\text{A}/\text{cm}^2$ respectively. Long-term tests at 1 V vs SCE showed that when the sample is illuminated for 4 hours, the current increases according to the equation $J = a \cdot \exp(-t/b) + c$, the value of the photocurrent was about 1 mA/cm². After this time, a change in current density was observed at a stationary potential also for 4 hours, the value of the current in this time range decreased according to the same equation. The b parameter was interpreted as reaction rate constant.

Based on the studies performed, it is assumed that the increase in current density during long-term tests at a potential of 1 V is associated with the formation of Fe(IV) on the surface of the photoanode. The formation of Fe(IV) is explained by the high concentration of holes at the photoanode/electrolyte interface due to the distribution of vacancies in the wall of the $\alpha\text{-Fe}_2\text{O}_3$ hollow sphere.

Audience Take-Away:

- The study is devoted to one of the most promising materials for photoanodes.
- The study talks about obtaining film with two-level structure.
- The study describes the photoelectrochemical behavior of films based on hollow microspheres and presents the relationship between the structure and properties of the material.

Biography

Alexander Demirov is a PhD student at the Department of Functional Nanosystems and High-Temperature Materials, National University of Science and Technology MISIS. In 2018, he received a master's degree in Materials Technology and Materials Science. His areas of interest are nanomaterials, functional coatings and electrochemistry. He has publications that are indexed in WoS and Scopus.



Shabanova Chimnaz Mamed

Azerbaijan National Academy of Science, Azerbaijan

Visual modeling of optimal regimes of chemical-technological process

Paper presents the results of modeling the optimal regime of the electrodeposition process of the antimony-selenium system Sb–Se. Based on the experimental data, a regression model was built using the BoxBenkinD module of the Matlab-7 software. The regression equation $Y = f(X_1, X_2, X_3, X_4)$ establishes the functional dependence of the product yield Y (in the form of deposition of the studied thin films of the Sb–Se antimony-selenium system) on 4 process parameters, where X_1 is the concentration of SbOCl in the range of 0.01–0.09 mol/l; X_2 - concentration of H_2SeO_3 (0.01–0.09 mol/l); X_3 - current density (20–60 mA/cm₂); X_4 - temperature (25–85°C). To solve the problem of process optimization, a specially developed by author software module was used. Restrictions are imposed on the objective function: $85\% \leq Y \leq 100\%$. To search for the optimal region, the parameters of one of the local maxima were chosen from the experimental data as the starting point. Start point coordinates: $X_1=0.09$, $X_2=0.01$, $X_3=20$ and $X_4=25$, $Y_{max}=87.5\%$.

In order to guarantee that the model provides high-precision predictions the regression analysis was implemented with the verification of the adequacy of the model (according to the Fisher criterion), as well as the study of the relative approximation error. The actual value of the Fisher distribution F-test: $F = 89.07$. Table value $F_t(4;11) = 3.36$. Since the actual value of $F > F_t$, and the average approximation error $\varepsilon = 1.11\%$, and thus regression characteristics are statistically significant it was concluded that the regression equation adequately describes this process.

Based on the constructed model, the response surface of the 2-parameter function $Y = f(X_1, X_3)$ was built, with fixed values of the parameters $X_2 = 0.01$, $X_4 = 25$ at the local optimum point and given intervals for X_1, X_3 . A specially developed software module is implemented in the Excel environment using Microsoft Excel add-in programs -VBA, Solver for optimization in what-if analysis. The module uses procedures to regulate, redirect of variable' cells content, which allows to conduct the calculations in interactive mode and get the distribution of function values at the response surface on an Excel sheet. In the set up stage conditions are introduced in the calculation mode to highlight the cells of the values of the objective function with a certain fixed color in the optimal area. Thus, the function calculation area filled with a pre-selected color visually identifies the optimal modes of the process.

As a result of applying the module under a given condition $85\% \leq Y \leq 98\%$ for the process, an optimal area was obtained with the following boundaries: $Y_{max} \in (85\% \div 97,9\%)$ at $X_1 \in (0.065 \div 0.089)$, $X_3 \in (20 \div 29)$, at $X_2 = 0.01$, $X_4 = 25$. For more precision conditions for the optimal yield of the product $92\% \leq Y \leq 98\%$, it was obtained: $Y_{max} \in (92.4\% \div 97.9\%)$ at $X_1 \in (0.078 \div 0.089)$, $X_3 \in (20 \div 23.5)$, at $X_2 = 0.01$, $X_4 = 25$.

Audience Take Away:

- Methods of identification of optimal regimes of chemical-technological processes
- Benefits of mathematical modeling for chemical-technological processes description
- Regression analysis application for verification of the adequacy of the model
- The advantages of mathematical modeling of a chemical process can be divided into economic-environmental and cognitive benefits. The main economic and ecological aspects of the advantages of modeling: reduced time spent on research; minimizing the use of consumables, reagents, toxic chemicals, devices used during the experiments; research costs are reduced. The benefits of a cognitive nature are associated with obtaining new information, knowledge about the process. An important function of the model is to identify the complexity of the process, to clarify the structure of the process or object under study, to streamline, highlight and identify new connections in the process under study. As a result, new ideas and a practical result should be proposed based on the model.

Biography

Ch. M. Shabanova studied Mathematics at the Baku State University, Azerbaijan and graduated as MS in 1982. She in 1984 joined the research group of Prof. R.M.Kasimov at the Institute of Catalysis and Inorganic Chemistry, Azerbaijan National Academy of Sciences (ICIC-ANAS) as senior researcher since 2004 and in 2016 joined the research group of Prof. M. Asadov at the same institution. She has published more than 40 research articles and theses. The main directions of scientific investigations: visual modeling of optimal areas for chemical-technological processes; visual mapping of phase diagrams of the multicomponent systems; polar liquids identification by construction of the polar liquid response surface using remote sensing method, development of pilot register of release and transfer of pollution (PRTR) from stationary sources in order to investigate the environmental pollution by toxic chemicals.

SPEAKERS
DAY 01

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16-17 **MAY**



Md Nurul Islam Siddique*, Zaiid bin Khalid

University Malaysia Terengganu, Malaysia

Bio-methane production from anaerobic digestion of agricultural waste with extra nutrients and intermediate temperature: Feasibility and fertilizer recovery

The rise in demand for organisms pulled in by anaerobic digestion might be due to the simultaneous digestion of many substrates. Supplements' effects on the co-digestion of growth substrates were investigated in this study. In three phases, 37 °C, 40 °C, and 50 °C, an additional improvement plan was utilised, which anticipates a crucial occupancy in anaerobic digestion. As a result of the adjustments, biogas output at 37 °C increased to 1.38 times that of the control. Furthermore, as a result of 40 °C without additives, an innovative philosophy was profoundly influenced by the good utilisation of this newly discovered mid-temperature (56 percent of VS end and 8.4 L-biogas) mL-CH₄/g-VS was 1.24 times that of the system without any further improvement during anaerobic co-digestion at 50 °C, and biogas production exceeded 11.3 L with supplements. The findings show that the modified course of action increases co-digestion at each temperature. On the advanced scale, the most commonly used temperature was 37 °C, which had the greatest impact on the use of improvements during the anaerobic process. Sludge was recovered from the digester at a rate of 0.09 m³ sludge/m³ substrate, whereas water was recovered at a rate of 0.86 m³ sludge/m³ substrate. The sludge that has been treated can be used as compost, and the water can be used to water plants. 3.77 years was discovered to be the time it took to repay the investment. As a consequence, it's possible that the present research may be acknowledged as a potential green option for waste management throughout the world in the near future.

Audience Take Away:

- Anaerobic digestion (AD) collects methane and provides a source of renewable energy that is carbon neutral i.e. provides energy with no net increase in atmospheric CO₂. Fertilizer - compared to undigested slurry, the nitrogen in digestate is more readily available as a plant nutrient.
- Farming waste production around the globe is up to 6 million tons yearly. From these wastes, those that originate from regular trade are yet disposed of in landfills and used for the ignition method with no treatment. This methodology, along these lines, prompts higher GHG emanations and environmental pollution. Anaerobic co-fermentation has been demonstrated to be a successful methodology for improved bio-methane generation from wastes. The mix of different substrates improves nutrition in the digestion system. Thus, microbes have access to supplemented media with an appropriate nutrient equalization. The fundamental targets of co-digestion ought to support valuable associations, keeping away from hindrance and upgrading methane generation. Yes, this research that other faculty could use to expand their research or teaching. Yes, this provides a practical solution to a problem that could simplify or make a designer's job more efficient. Yes, it improves the accuracy of a design or provides new information to assist in a design problem. all other benefits are listed below:
- Improved hydrolysis, pathogen removal, and minimum odor are the key benefits of a thermophilic run.
- On the other hand, the mesophilic run saves energy and is not affected by shock loading than a thermophilic run.
- Besides, a vast microbial community is estimated under a mesophilic state that may help to digest numerous types of organic substances.
- The thermophilic state helps the elimination of pathogens and produces enhanced methane. Nevertheless, the use of intermediate temperatures has not been studied deeply which can influence the system.
- The related works found in the literature didn't study the gap between the feasibility study and fertilizer recovery. Therefore, our work is novel and has detailed data and explanations on the feasibility study and fertilizer recovery.

Biography

Dr. Md Nurul Islam Siddique studied Civil Engineering at the Khulna University of Engineering & Technology, Bangladesh, and graduated as MS in 2012 from University Malaysia Pahang. He then joined the research group of Prof. Zularisam at the Institute of University Malaysia Pahang. He received her Ph.D. degree in 2015 at the same institution. After that, he obtained the position of Assistant Professor at the University Malaysia Pahang. She has published more than 40 research articles in ISI journals.



Víctor Cerda

University of the Balearic Island, Spain

Kinetic methods in analytical chemistry

A review of different analytical methods, from classical up to current automatic kinetic-catalytic methods using chip systems, will be presented

Background of the kinetic methods of analysis. How to use the different kinetic-catalytic methods: fixed time, fixed measure and initial-rate methods. Simultaneous determinations of the catalysts and activators. Automatic kinetic and kinetic-catalytic methods of analysis. Use of in-chip catalytic methods

Audience Take Away:

- Yes. This review will help what to explain the kinetic methods in classroom
- The review will include a lot of examples how the kinetic and kinetic catalytic methods have been applied using different measuring techniques

Biography

Dr. Víctor Cerdà studied Chemistry at the Barcelona University. He joined the research group of Prof. Francisco Buscarons at the Analytical Chemistry Department. He received his PhD degree in 1973 at the same institution. He obtained the position of a Full Professor in the University of the Balearic Island, where he was head of the Chemistry Department, Vice-chancellor of Scientific Policy, Founder and President of the Association of Environmental Analytical Chemistry and of the Sciware Systems as a Spin Off company of this university. He has published 14 books, more than 600 research articles in SCI (E) journals, and more than 800 contributions in international conferences.



Andrea Czompa* and I. Mándity

Semmelweis University, Hungary

Propylene carbonate in Suzuki-Miyaura reaction

Several efforts were taken to carry out cross-coupling reaction under green and sustainable conditions. The Pd-catalysed cross-coupling of three iodo-heterocyclic compounds with different boronic acids will be discussed under Suzuki-Miyaura reaction conditions, in a green solvent. The propylene carbonate (PC) is a polar, aprotic solvent synthesized by addition of propylene oxide to carbon dioxide. It has a high boiling point and is more or less stable at elevated temperatures. This property of PC allows the Suzuki-Miyaura reaction to be carried out at higher temperatures, but under a shorter reaction time.

In the presence of base, PC suffers ring-opening and the formed propylene-glycol is able to alkylate the nucleophilic N-heteroatom giving byproducts with 2-hydroxypropyl side-chain besides the expected coupled products. We compared the yield of products obtained by traditional oil-heating with those obtained under similar reaction conditions under microwave irradiation as well. In some cases, the reactions were performed under flow conditions too. Based on the results, we assume that there are two possibilities: alkylation takes place first and then cross coupling happens or vice-versa. The first option was verified according to our investigation.

In sum, a green procedure was developed not only for the Suzuki-Miyaura cross-coupling reaction, but N-alkylation was carried out under sustainable conditions providing compounds not known in the literature, which possess a free OH-group and which may lead to the synthesis of drug candidates after further transformations.

Biography

Dr. A. Czompa studied Chemistry at the Babes-Bolyai University, Romania and graduated as chemistry-physics teacher in 1993. She joined the research group of Prof. S. Antus at the Department of Organic Chemistry, University of Debrecen. She received her PhD degree in 2000 at the same institution, in the field of flavonoid derivatives, enzymatic reaction and SAR. After moving to Budapest, at Semmelweis University she continued to deal with organic chemistry and synthesized pyridazinone ethers, glycine transporter-1 inhibitors, optical BAPTA-derivatives, antiarrhythmic compounds, SSAO/VAP-1 inhibitors, TRPA1 and V1 receptor antagonists, SzV-1287 and metabolites, respectively new N-, O-, S-heterocyclic compounds.



Bruno Mattia Bizzarri*, Angelica Fanelli, Lorenzo Botta, Marta De Angelis, Anna Teresa Palamara, Lucia Nencioni, Raffaele Saladino

University of Tuscia, Italy

Aminomalononitrile and Diaminomaleonitrile inspired prebiotic chemistry as a novel multicomponent tool for the synthesis of imidazole purine and pyrimidine derivatives

Amino imidazole carbonitrile derivatives decorated with α -amino acid side-chains have been synthesized by a multicomponent microwave assisted reaction inspired by the prebiotic chemistry of aminomalononitrile as a tool for generating high chemical diversity. These compounds were used as annulation synthons for the preparation of 8,9- disubstituted-6,9-dihydro-1H-purin-6-ones by reaction with formic acid as a simple C-1 donor reagent. The novel heterocycles were characterized by significant activity against influenza A virus, amino imidazole carbonitrile derivatives showing the highest activity. Thus, the chemical complexity generated by prebiotic chemistry furnished a general tool for the identification of novel antiviral agents.

Audience Take Away:

Today, the modernization of the MCC by innovative techniques (e.g. microwave-assisted procedures) furnishes an impressive combination of tools to force and speed-up the production of complex heterocyclic derivatives encompassing the so called "Molecular Evolution-Inspired Synthesis". In this context, aminomalononitrile (AMN) has been identified as a common intermediate in the prebiotic chemistry of HCN and NH_2CHO , besides to diaminomaleonitrile. AMN is involved in the formation of imidazole intermediates, such as amino imidazole carbonitrile and amino imidazole carboxamide, which are precursors of purine and pyrimidine nucleobases and analogues. The presentation will be focused on an innovative multicomponent prebiotic chemistry approach for the preparation of amino imidazole carbonitrile and purine derivatives decorated with different α -amino acid side-chains. The synthesis involves a one pot microwave-assisted condensation followed by a solvent free annulation and represent the first link between prebiotic chemistry and modern viruses.

Biography

Bruno Mattia Bizzarri is Post-Doc researcher and a professor of Organic chemistry at the Department of Ecology and Biology, University of Tuscia. In 2013 he was graduated in Medicinal Chemistry at University of Siena and he received the Ph.D. degree in Green Chemistry in 2017. His research work is mainly focused on the synthesis of natural products by the application of new green chemistry approaches and the investigation of prebiotic chemistry processes in a chemo mimetic view. In particular, he is mainly involved in the development of a multicomponent synthesis for the preparation of selected bioactive compounds starting from prebiotic probe.



Mohamed Ezeldin Osman*, V. V. Maximov, T.F. Sheshko, A.G. Cherednichenko, V.M. Kogan

Peoples' Friendship University of Russia, Russia

Syngas conversion into higher alcohols over KCoMoS₂-catalysts supported on graphene-nanosheets coating alumina and carbon-containing materials

Catalytic conversion of synthesis gas to higher alcohols has received tremendous interest due to the generation of environmentally benign octane boosters and alternative fuels to supplement the diminishing supply of the world's finite fossil fuel reserves. K-modified CoMoS₂ catalysts supported over carbon-containing materials such as γ -Al₂O₃, Carbon-Coated Alumina (CCA), Graphene coated Alumina (GCA), and different types of powdered and fiber commercial activated carbons were prepared and characterized by BET, XRF, SEM, SEM-EDX, and HRTEM. Supporting efficiency of γ -Al₂O₃ to synthesis alcohols from syngas via KCoMoS₂ catalyst improves after being coated with amorphous carbon and graphene because the carbon materials played a role in decreasing the interaction between alumina and active phase besides it has decreased the hydrogenation reaction. Powdered and fiber commercial activated carbons have shown different activities to increase the yield and selectivity of alcohol products. The catalytic activity increased in the order TCA < OBC-1 < DAC < AHM < AG-3 < BAW. It was found that catalysts supported on microporous materials possessed higher catalytic activity in HAS synthesis from syngas than mesoporous materials. We explained this phenomenon by the distribution of the active phase inside the pores and the catalyst acidity. These results give deeper insight into the catalyst design of supported- TMS for HAS.

Biography

Dr. Osman studied Chemistry at Omdurman Islamic University, Sudan, and graduated as M.Sc. in 2015. He received his PhD degree in 2018 at Sudan University of Science & Technology, Sudan. In the same year, he started his second PhD in Physical Chemistry at Peoples' Friendship University of Russia, Russia under the co-supervision of Prof. V.M. Kogan and Prof. T.F. Sheshko. He then joined the research group of Prof. Victor Kogan at N.D. Zelinsky Institute of Organic, Russia Academy of Sciences (RAS). Also, He is working at RUDN University in the Full Employment PhD Program.



Elisabete Alegria*, Guilherme Marques, Mohamed Soliman, Manas Sutradhar, Daniela Flores, Carlos Granadeiro, Salete S. Balula, João Pires, Armando Pombeiro

Instituto Superior de Engenharia de Lisboa, Portugal

Vanadium(V) complexes supported on porous MIL100(Fe) as catalyst for the peroxidative oxidation and adsorption of VOCs

In this work, the vanadium(V) complexes bearing the aroylhydrazone Schiff base 2-hydroxy-N'-((2-hydroxynaphthalen-1-yl)methylene)benzohydrazide ligand, $[\text{VO}(\text{OMe})\text{L}]$ (1) and $[\text{Et}_3\text{NH}][\text{VO}_2\text{L}]$ (2) were synthesized, characterized and supported on porous MIL-100(Fe) MOF via an impregnation method forming the 1@MIL-100(Fe) and 2@MIL-100(Fe) composites. The immobilization of the vanadium compounds on MIL-100(Fe) was assessed by several characterization techniques, namely powder X-ray diffraction, UV/Vis, FTIR, SEM-EDS, ICP and BET surface area analysis, confirming the successful heterogenization of both vanadium complexes. Both complexes were screened as catalysts towards the oxidation of toluene, under homogenous (1 and 2) and heterogeneous (1@MIL-100(Fe) and 2@MIL-100(Fe)) conditions as well as for toluene adsorption. For the catalytic oxidation of toluene, the influence of several parameters such as type and amount of catalyst, type and amount of oxidant, reaction time, temperature, radical trapping and catalyst recycling (for heterogenous) was studied. Benzaldehyde, benzyl alcohol and benzoic acid were identified as the main products.

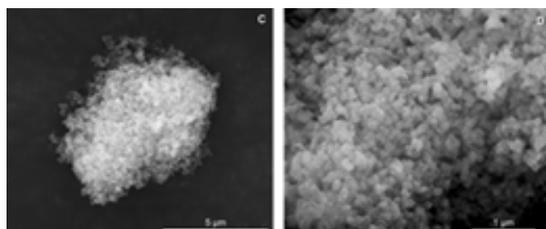


Fig. 1 - SEM images of 2@MIL-100(Fe).

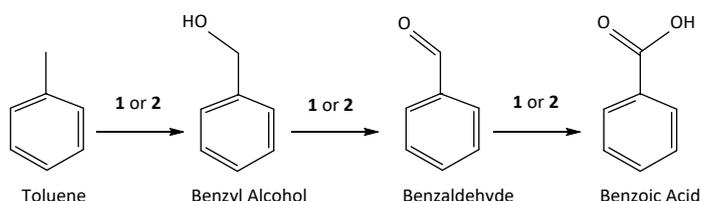


Fig. 2 - Peroxidative oxidation of toluene by 1 or 2.

Audience Take Away:

- Volatile Organic Compounds (VOCs): emission and risks;
- Available techniques for VOCs removal/control
- Catalytic Oxidation of VOCs as promising strategy
- Supported Catalysis

Biography

Elisabete Alegria got her Ph.D degree (2006) from Instituto Superior Técnico, University of Lisbon. She is Researcher (Core Member) at Centro de Química Estrutural (Coordination Chemistry and Catalysis Group) at Instituto Superior Técnico since 2009. She was appointed as Adjunct Professor (2007) at the Chemical Engineering Department of Instituto Superior de Engenharia de Lisboa (ISEL) from Polytechnic Institute of Lisbon. E.C.B.A. Alegria authored over 80 scientific papers, 4 patents, 3 book chapters, and over 100 scientific communications.

Main research interests: Sustainable homogeneous and supported catalysis for VOCs conversion and Biomass valorization, green synthesis of metallic nanoparticles, mechanochemistry (synthesis and catalysis), molecular electrochemistry.



Rupesh Hiranman Gaikwad

Maharshi Dayanand College, India

Advances in metal oxide and mixed metal oxide catalysis and their applications

Metal oxide catalysts are much more complicated than metal catalysts. The reason is that the cations of the metal atoms could exhibit a few different oxidation states on surface of the same catalyst particle or change of their oxidation states under different reactive environments. The complication of surface chemistry and structure of a metal oxide makes studies of surface of an oxide catalyst very challenging.

The present article contains the fundamentals of heterogeneous catalysis and a description of the main domains of heterogeneous catalysis in metal oxide and mixed metal oxide catalysts and also considers current and prospective major applications, where recent advances in the science of metal oxide catalysts have major economic and environmental impacts.

Metal oxides are utilized both for their acid–base and redox properties and constitute the largest family of catalysts in heterogeneous catalysis. A variety of metal oxide and mixed metal oxides (MMOs), containing alkali, alkaline, rare earth and noble metals, and their applications are presented.

Keywords: metal oxide catalysts, mixed metal oxide catalyst, heterogeneous catalysis,

Audience Take Away:

- The presentation will help them to develop a faculty in the metal oxide catalysis and they can use the presentation as a base for the primary studies.
- This presentation will help the participant to generate ideas which can be utilized in their respective fields. Even the researcher can explore the research on this foundation. Even the tailor-made design of the metal oxide can help in exploring applications in different areas where specific designs of the catalyst is required.

Biography

Dr. Rupesh H. Gaikwad, post graduated in Inorganic Chemistry in 2004 and after a stint in academic and industry for 2 years he joined the research group of Dr. R. V. Jayaram, at Institute of Chemical Technology, Mumbai, India and received PhD degree in 2014, while working on topic of nitrogen and phosphorous based extractants for nuclear fuel reprocessing. Then in 2015 he joined as Assistant Professor, Department of Chemistry, Maharshi Dayanand College, Mumbai, India. He is an executive committee member of National Centre for Science Communicators India, and delivered talks on science popularization amongst students and general public. He is appointed as member of Science World Encyclopedia, which will be written in regional (Marathi) language , by Government of Maharashtra, India.



Sujoy Bandyopadhyay

Indrashil University, India

Conjugated porous organic polymers: Fluorescence-based sensing, photocatalysis and energy storage

Starting from the grand old activated charcoal to zeolites, porous materials have been utilized for environmental and technological benefits for mankind. Of late, porous organic polymers (POPs) have emerged as a new class of functional materials with applications ranging from gas adsorption, gas/liquid separations, catalysis, light harvesting to chemo/biosensing. A combination of porosity and π -electron conjugation leads to the development of a new field of conjugated porous organic polymers (CPOPs). In this context, we have designed a new core of tetraphenyl-5,5-dioctylcyclopentadiene (TPDC), and fabricated CPOPs in the form of solid, soluble in organic solvents and nanoparticles. The soluble CPOP and the aqueous dispersion of nanoparticles employed for nitroaromatics sensing by amplified fluorescence quenching. Tunable surface area and fluorescence were achieved in TPDC-based polymers by varying the comonomers and polymerization conditions. Mesoporous to ultra-microporous CPOPs with surface area 73 to 1010 m²g⁻¹ were fabricated using 4,4-difluoro-4-bora-3a,4a-diaza-s-indacenes (BODIPY) core and explored for catalytic photooxidation of thioanisol. Further, the systematic investigations with a series of heteroatom containing CPOPs led to the construction of pyrene and 4,4'-diaminobiphenyl based CPOP with specific capacitance \sim 456 Fg⁻¹ at 1 mv s⁻¹ scan rate. Addressing the cardinal issue of solution processability, a general design principle is also presented in the thesis with a special emphasis on carbazole-BODIPY based CPOPs for visible-light-driven reactive oxygen species (ROS)-mediated metal-free organic transformation.

Audience Take Away:

- In this talk I will explain how soluble porous organic polymer (POPs) can be synthesized
- Multifunctional application of POPs as well how we can tune the porosity and surface area of the POPs .

Biography

Dr. Sujoy Bandyopadhyay earned his MS in Chemistry from Vidyasagar University in India. He later joined Prof. Abhijit Patra's research group at the Indian Institute of Science Education and Research in Bhopal. He obtained his PhD from the same university in 2018. After completing a one-year postdoctoral programme at Hanyang University under the supervision of Prof. Hyosung Choi, he was hired as an Assistant Professor at Indrashil University. He has about 15 research publications published in SCI(E) journals.



Mridusmita Barooah

National Institute of Technology, India

Mixed matrix membrane for high CO₂ gas performance studies

Contemporary advances in materials development associated to the gas separation technology refers to the cost-effective fabrication of high performing defect free mixed matrix membranes. Being proven to be effective for cleaner energy production, natural gas purification and CO₂ capture from flue gas systems, the mixed matrix membranes constitute the functional integration of polymer matrices (performing within the trade-offs of Robeson's plot) and mostly inorganic filler materials (performing beyond the Robeson's plot-based trade-offs). The broad domain of MMM research and development devotes towards selection of appropriate materials, defect free inexpensive fabrication and characterization for simulated and real-world application scenarios. A comprehensive review in the state-of-the-art of MMMs has been addressed in this article. The material selection related aspects have been discussed in the context of polymer and filler particle morphology and compatibility. Thereafter, the relevance of several inorganic fillers in various MMMs has been compiled and analysed. Eventually, modelling approaches have been summarized for the evaluation of MMM's gas separation characteristics. A critical feature of the article is to devote towards possible remedial actions in due course of the achievement of a high performing defect free MMMs. Finally, the article devotes towards possible scope for furthering the existing challenges and characteristics of the MMMs.

Audience Take Away:

- This article provides a comprehensive review with respect to the utility of MMMs (constituting a bulk and a filler scattered phase) towards CO₂ separation. A thorough analysis was carried out with respect to the filler particles in the MMM and their ability to enhance the CO₂/N₂ gas transport properties.
- This study provides alternate advanced fabrication methods to achieve MMMs with high performance in gas separation.
- Modifying agents have been added to improve the physico-chemical properties of the membrane. As indicated, the size, shape and porosity of the filler particles significantly influence the gas separation characteristics of the MMMs. Characterization studies concluded that the functionalization agents improve the membrane performance.
- The high-end separation technology provided opportunity for large-scale gas separation operation and a very viable approach to be replaced with the conventional separation technology in terms of physico-chemical property enhancement and gas separation performance.

Biography

Dr. Mridusmita Barooah did her graduation in Chemical Engineering from Assam Engineering College, Guwahati, Assam in 2012. Thereafter, she worked as Project Scientist in DST sponsored projects, Government of India from CSIR-North East Institute of Science and Technology, Jorhat and Indian Institute of Technology (IIT) Guwahati. She then joined the research group of Dr. Bishnupada Mandal, Senior Professor, Department of Chemical Engineering, IIT Guwahati. She was awarded her PhD degree in 2019. Her PhD topic was, "Development of CO₂ selective mixed matrix membrane for CO₂ separation." She worked in National Institute of Technology (NIT), Arunachal Pradesh as Assistant Professor from July 2019 and has taught core subjects in Chemical Engineering which include Mass Transfer, Chemical Reaction Engineering, Chemical Process Technology, Process Instrumentation, Chemical Engineering lab. She is currently working as Assistant Professor, NIT Warangal, Telangana, India. She has 4 International publication of research article and attended many International and national conference along with workshops.



Rabeharitsara Andry Tahina,

Polytechnic Engineer School of Antananarivo University, Madagascar

Trans-esterification with methanol of *Capscicum Chinense's* citric acid ester solution – Its calcium gel and crystal salts synthesis

First, it will be presented in this communication the procedure, the experimental conditions and the results of the *Capscicum chinense* esterification with citric acid molecules catalysed by the protonic acid-H⁺ of these citric acid molecules. Then, these synthesized esters was valorised to calcium gels and crystals salts by adding calcium hydroxide. Indeed, a procedure of this valorisation was established deduced by an investigation of the reactions between the citric acid esters and calcium hydroxide and each equivalent products structure. The characterisations of the gels and crystals salts by the EDTA-0.01N complexometric titration procedure permitted not only to determine their calcium concentrations but also to realize that the synthesized structure -O-Ca-O- was stable. In addition, their titrations by the HF-0.0026N procedure permitted to confirm and to quantify their alkene organic function obtained by dehydration reaction catalysed by the protonic acid-H⁺ of citric acid molecules.

Second, seeing that this esterification with citric acid molecules permitted to extract the raw materials molecules, a trans-esterification with methanol of this citric acid ester solution followed by hexane and dichloromethane extraction procedures was established in order to analyse with high performance liquid chromatography-hplc the principal molecules of the raw material and its synthesized derivatives. In this case of *Capscicum chinense* as raw material, it was confirmed the presence of luteolin, capsaicinoides, quercetin and flavonoids, amines molecules with their derivatives obtained by trans-esterification with methanol of the *Capscicum chinense's* citric acid esters solution.

Noticed that these previous studies contributed not only for the characterizations of the spices-raw material but also their valorization as spices' citric acid esters calcium gels/crystals salts and as energy booster like our spicy product energy booster speb-pebe products.

Audience Take Away:

- Synthesis of raw materials' citric acid esters solutions.
- Valorization of raw materials' citric acid esters to their equivalent calcium gels and crystals salts.
- Trans-esterification with methanol of raw materials' citric acid esters solutions followed by the extraction with dichloromethane and hexane of this previous trans-esterification products.
- Analysis on high performance liquid chromatography-hplc of the *Capscicum chinense's* (could be expanded to other raw materials') dichloromethane extracted molecules and possible analysis on gas chromatography-cpg of its hexane-fatty acids and derivatives extracted molecules.
- Spicy product energy booster / speb-pebe products.

Biography

Dr. Rabeharitsara Andry Tahina studied Chemistry at the Polytechnic Engineer School of Antananarivo University and graduated as Chemical Engineer in 1999. He then joined the research group of Prof. Michel Guisnet and Patrick Magnoux at the LACCO-UMR 6503-Poitiers University until getting the PhD degree of Applied Organic Chemistry on zeolite acid catalysis in 2003. After getting the Master's degree of business administration at the IAE institute of Poitiers-University, he got the position of Assistant Professor at the Antananarivo Polytechnic Engineer School/Chemical Engineering department from 2008 where he has published 15 research articles in the American Journal of Applied Chemistry.

KEYNOTE FORUM

DAY 02

11TH EDITION OF
INTERNATIONAL CONFERENCE ON
**CATALYSIS, CHEMICAL
ENGINEERING AND
TECHNOLOGY**

16-17 MAY

**Osman Adiguzel**

Firat University, Turkey

Lattice reactions governing thermoelasticity and superelasticity in shape memory alloys

Some materials take place in class of smart materials with adaptive properties and stimulus response to the external changes. Shape memory alloys take place in this group by exhibiting dual thermoelastic and Superelastic characteristics. These alloys have shape reversibility at different conditions and shape of material cycled between original and deformed shapes at different condition. Shape memory effect is initiated by cooling and deformation the material and performed thermally on heating and cooling after first cooling and stressing treatments. Therefore, this behavior is called thermoelasticity. Superelasticity is another property and performed in only mechanical manner. These alloys can be deformed in parent phase region just over austenite finish temperature and recover the original shape on releasing the external forces. These phenomena are result of crystallographic transformations in the materials, called martensitic transformations. Shape memory effect is governed by successive thermal, and stress induced martensitic transformations. Thermal induced martensitic transformations occur on cooling with cooperative movement of atoms by means of lattice invariant shears in $\langle 110 \rangle$ - type planes on $\{110\}$ - type planes of austenite, along with lattice twinning and ordered parent phase structures turn into twinned martensite structures; these twinned structures turn into detwinned martensite structures by means of strain induced martensitic transformation with deformation in martensitic state. Superelasticity is also the result of stress-induced martensitic transformation, and parent austenite phase structures turn into the fully detwinned martensite with the stressing. Superelasticity exhibits normal elastic material behavior, but it is performed in non-linear way; loading and unloading paths are different, and hysteresis loop reveals energy dissipation. Copper based alloys exhibit this property in metastable β - phase region, which has bcc-based structures at high temperature parent phase field. Lattice invariant shear and twinning is not uniform in copper alloys and they give rise to the formation of unusual layered complex structures, like 3R, 9R or 18R structures depending on the stacking sequences, with lattice twinning. The unit cell and periodicity is completed through 18 layers in direction z, in case of 18R martensite, and unit cells are not periodic in short range in direction z.

In the present contribution, x-ray diffraction and transmission electron microscopy studies were carried out on two copper based CuZnAl and CuAlMn alloys. X-ray diffraction profiles and electron diffraction patterns exhibit super lattice reflections inherited from parent phase due to the displacive character of martensitic transformation.

Keywords: Martensitic transformation, shape memory effect, thermoelasticity, superelasticity, lattice twinning, detwinning.

Audience Take Away:

- Shape memory alloys are multifunctional materials and used as shape memory devices from biomedical to every field of engineering.

Biography

Dr Adiguzel graduated from Department of Physics, Ankara University, Turkey in 1974 and received PhD- degree from Dicle University, Diyarbakir-Turkey. He has studied at Surrey University, Guildford, UK, as a post-doctoral research scientist in 1986-1987, and studied on shape memory alloys. He worked as research assistant, 1975-80, at Dicle University and shifted to Firat University, Elazig, Turkey in 1980. He became professor in 1996, and he has already been working as professor. He published over 60 papers in international and national journals; He joined over 100 conferences and symposia in international and national level as participant, invited speaker or keynote speaker with contributions of oral or poster. He served the program chair or conference chair/co-chair in some of these activities. In particular, he joined in last seven years (2014 - 2020) over 80 conferences as Keynote Speaker and Conference Co-Chair organized by different companies. He supervised 5 PhD- theses and 3 M.Sc.- theses. Dr. Adiguzel served his directorate of Graduate School of Natural and Applied Sciences, Firat University, in 1999-2004. He received a certificate awarded to him and his experimental group in recognition of significant contribution of 2 patterns to the Powder Diffraction File – Release 2000. The ICDD (International Centre for Diffraction Data) also appreciates cooperation of his group and interest in Powder Diffraction File.



Tokeer Ahmad

Jamia Millia Islamia, India

Designing nanocatalysts for H₂ energy generation and heterogeneous organic transformation reactions

Multifunctional nanostructures find the possibility for their applications in water splitting processes for hydrogen generation as a renewable source of green energy. Fe₃O₄ nanocubes were prepared in one pot process for the electrochemical water splitting and supercapacitor applications. As-synthesized Fe₃O₄ nanocubes with high specific surface area of 268 m²g⁻¹, are ferromagnetic at room temperature and affects the electro-catalytic activity of the electrode materials. Similarly, the catalytic activity of ultrafine nanoparticles was examined against the Horseradish peroxidase enzyme and applied as sensor for the detection of H₂O₂ in the solution. Besides that, the stimulating bifunctional electro-catalytic performance of RuO₂ nanoparticles was studied under different atmospheric conditions for electrochemical hydrogen energy. The studies of some multifunctional nanoparticles by citrate precursor route reveal the formation of monophasic nanostructures with fairly uniform distribution of nearly spherical particles, high specific surface area and visible optical band gap. Photocatalytic generation of hydrogen in water splitting process by using as-prepared nanoparticles has also been studied under the visible light irradiations which showed a significant H₂ evolution reaction rate. The development of nanostructured catalysts has also been preferred to carry out the heterogeneous catalytic organic transformations because of greater number of surface-active sites for catalytic processes, high catalyst recovery rate, especially their environment friendly nature and their ease of synthesis. Besides the advances in nanocatalysis, certain challenges including not well-defined morphologies due to loss of control over it and loss of catalytic activity during operation need to be addressed. Herein, we discuss some nanocatalysts for certain organic transformation reactions with enhanced activity.

Audience Take Away:

- The presentation will be useful to get break through and idea for new problems for young researchers.
- The researchers will get lecture training to use nanomaterials for hydrogen production.
- The researchers can use our strategy for organic conversion reactions.
- Industrially very important topics under nanocatalysis.

Biography

Prof. Tokeer Ahmad did his masters from IIT Roorkee and Ph.D. from IIT Delhi. Presently, he is full Professor at Jamia Millia Islamia, New Delhi. Prof. Tokeer Ahmad has supervised 9 PhD's, 71 postgraduates, 9 research projects, published 117 research papers and two books with research citation of 3825, h-index of 36 and i10-index of 77. Prof. Ahmad is active reviewer of 103 journals, delivered 89 Invited talks and presented 120 conference papers. Prof. Ahmad has received DST-DFG award, ISCAS Medal, Inspired Teacher's President Award, Distinguished Scientist Award and elected as Member of National Academy of Sciences India. Prof. Ahmad has been figured in World Top 2% Scientists by Stanford University, USA and has been recently conferred the prestigious Maulana Abul Kalam Azad Excellence Award of Education for the outstanding contribution in the field of education.



Alexander G. Ramm

Kansas State University, United States

Solution of the millennium problem concerning the navier-stokes equations

The Navier-Stokes problem in \mathbb{R}^3 consists of solving the equations: $v^0 + (v, \nabla)v = -\nabla p + \nu \Delta v + f$, $x \in \mathbb{R}^3$, $t \geq 0$, $\nabla \cdot v = 0$, $v(x, 0) = v_0(x)$, where $v = v(x, t)$ is the velocity of the incompressible viscous fluid, $p = p(x, t)$ is the pressure, the density of the fluid is $\rho = 1$, $f = f(x, t)$ is the exterior force, $v_0 = v_0(x)$ is the initial velocity.

The aim of this talk is to analyse the Navier-Stokes problem (NSP) in \mathbb{R}^3 without boundaries. It is proved that the NSP is contradictory in the following sense: If one assumes that the initial data $v(x, 0) \not\equiv 0$, $\nabla \cdot v(x, 0) = 0$ and the solution to the NSP exists for all $t \geq 0$, then one proves that the solution $v(x, t)$ to the NSP has the property $v(x, 0) = 0$.

This paradox (the NSP paradox) shows that the NSP is not a correct description of the fluid mechanics problem for incompressible viscous fluid and the NSP does not have a solution defined for all $t > 0$. In the exceptional case, when the data are equal to zero, the solution $v(x, t)$ to the NSP does exist for all $t \geq 0$ and is equal to zero, $v(x, t) \equiv 0$.

These results are proved in [1]–[4].

These results solve one of the millennium problems.

Key words: The Navier-Stokes problem

Biography

Alexander G. Ramm was born in Russia, emigrated to USA in 1979 and is a US citizen. He is Professor of Mathematics with broad interests in analysis, scattering theory, inverse problems, theoretical physics, engineering, signal estimation, tomography, theoretical numerical analysis and applied mathematics. He is an author of 708 research papers, 20 research monographs and an editor of 3 books. He has lectured in many Universities throughout the world, gave more than 150 invited and plenary talks at various Conferences and had supervised 11 Ph.D students. He was Fulbright Research Professor in Israel and in Ukraine, distinguished visiting professor in Mexico and Egypt, Mercator professor, invited plenary speaker at the 7-th PACOM, he won Khwarizmi international award in 2004, and received many other honors. A.G.Ramm has solved inverse scattering problems with fixed-energy scattering data, with non-over-determined scattering data and studied scattering problems with under-determined scattering data. He solved many specific inverse problems and developed new methods in this area. He solved the many-body wave scattering problem when the bodies are small particles of arbitrary shapes and used this theory to give a recipe for creating materials with a desired refraction coefficient. These results attracted attention of the scientists working in nanotechnology. He gave formulas for the scattering amplitude for scalar and electro-magnetic waves by small bodies of arbitrary shapes and formulas for the polarizability tensors for such bodies. He gave a solution to the Pompeiu problem, proved the Schiffer's conjecture and gave first symmetry results in harmonic analysis. He has developed the Dynamical Systems Method (DSM) for solving linear and non-linear operator equations, especially ill-posed. He developed a random fields estimation theory and studied convolution equations with hyper-singular integrals. recently, he solved the millennium problem, the Navier-Stokes problem (NSP) and proved a paradox in the NSP which shows the contradictory nature of the NSP and the non-existence of its solution on the interval $t \in [0, \infty)$ for the initial data $v_0(x) \not\equiv 0$ and $f(x, t) = 0$.



Anne M. Gaffney

University of South Carolina, Columbia, South Carolina, USA

New perspectives and insights into silver catalyzed direct propylene epoxidation

A series of Ag-based catalysts were studied for direct PO epoxidation with O_2 as the oxidant. Ag supported on $CaCO_3$ and $\alpha-Al_2O_3$ were prepared as base materials to study. Promoters (K^+ , Cs^+ , Mo) and feed additives (EtCl, NO, CO_2) were added to the catalyst and feed stream, respectively, in order to evaluate their effects on PO selectivity and yield. Ball-milling of the catalyst during preparation was a significant factor in ensuring proper blending of promoter species in the Ag particle. Surface characterization (chemisorption, XPS, SEM-EDX), bulk composition characterization (XRD, ICP-OES), and reaction kinetic evaluation were conducted to understand the nature of PO selectivity.

Biography

Dr. Anne M. Gaffney is the Chief Science Officer of Idaho National Laboratory and Distinguished National Lab Fellow (2014 – present). She has thirty-four years of experience working in industry inventing and commercializing new technologies for major chemical manufacturing companies including Koch Industries, Lummus Technology, Dow, Dupont and ARCO Chemical Company. She has authored 155 publications and 256 patents. Dr. Gaffney is also a distinguished Joint Appointment Fellow at the University of South Carolina (2018 – present) where she is the Technical Director of the National Science Foundation Center for Rational Catalyst Synthesis. Some of her recent awards include: the 2019 American Chemical Society, Energy & Fuels, Distinguished Researcher Award in Petroleum Chemistry; the 2015 Eugene J. Houdry Award of the North American Catalysis Society; the Chemical Heritage Foundation, Women in Science Inductee, 2014; and the American Chemical Society, Industrial Chemistry Award, 2013. Dr. Gaffney received her BA in chemistry and mathematics from Mount Holyoke College and her Ph.D. in physical organic chemistry from University of Delaware.



P. Szuroczki, A. Takács, and L. Kollar*

University of Pecs, Hungary

Functionalization of N-Heterocycles in transition metal catalyzed reactions

There are several ways of introducing acyl functionality into simple model compounds or skeletons of practical importance. The application of conventional acylating agents is well known and is referenced in reviews, handbooks and even textbooks. Since the discovery of the aminocarbonylation by Heck *et al* ('Heck-carbonylation'), the use of a primary or secondary amine, carbon monoxide and aryl/alkenyl halides (or their synthetic surrogates, silyl triflates and alkenyl triflates) in the presence of palladium catalysts lead to carboxamides in great variety.

Our presentation will be focused on the following topics:

- The efficiency of palladium(II)-acyl intermediates, formed via carbon monoxide insertion into Pd-aryl/alkenyl bonds, as acylating agents will be exemplified.
- The reaction mechanism will be rationalised on the basis of a catalytic cycle.
- High-yielding palladium-catalysed aminocarbonylation of functionalised iodoaromatics and iodoalkenes towards carboxamides (via single CO insertion) and 2-ketocarboxamides (via double CO insertion) will be discussed. The functional group tolerance of the palladium-catalysed reaction will be shown.
- The synthesis of compounds of pharmacological importance (penicillins, cephalosporins, etc.) will be discussed by choosing more complicated skeletons as N-nucleophiles in aminocarbonylation.
- The efficiency of the combination of high-yielding conventional reactions and highly selective homogeneous catalytic reactions will be shown in multistep syntheses under green conditions.

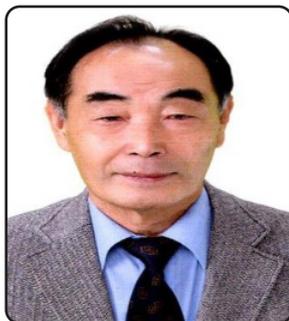
Biography

Laszlo Kollar received his diploma in 1979 and the doctoral degree in 1983 at the University of Veszprém, Hungary. He is now the Head of the Institute of Chemistry at the University of Pécs, Hungary. The main efforts of his current research are focused on the synthetic application of transition metal complexes regarding the functionalization of steroids and N-heterocycles of pharmacological importance, as well as PARP inhibitors. He is the author of more than 300 papers published in international journals and co-author of 9 basic patents on 5 α -reductase inhibitors and agrochemicals.

SPEAKERS
DAY 02

**11TH EDITION OF
INTERNATIONAL CONFERENCE ON
CATALYSIS, CHEMICAL
ENGINEERING AND
TECHNOLOGY**

16-17 **MAY**



Dai-Yeun Jeong

Jeju National University, Korea

A desirable approach to establishment of climate change policy

There are four major agents responding to climate change at a national or local level. They are government, enterprises, citizens and civil organizations. Government responds to climate change by establishing policies, enterprises by green management for improving eco-efficiency in the process of producing and distributing goods and services, citizens by eco-friendly behavior in their everyday life, and civil organizations by environmental movement.

This paper presents a desirable approach to the establishment of climate change policy by government in order of the following four stages.

The 1st stage is to identify the vulnerability to climate change. A desirable conceptual framework for identifying the vulnerability will be presented.

The 2nd stage is what should be considered for establishing policies on the basis of the vulnerability identified from the first stage. This stage will present how to select the prior vulnerable sectors as the targets of policy formulation, how to set up the goal of vulnerable sector to achieve, and what means to mobilize to achieve the goal.

The 3rd stage is what type of governance system should be introduced in the process of establishing policies. This stage will present desirable phases of governance system being employed in the process of establishing optional policies for drawing a social consensus.

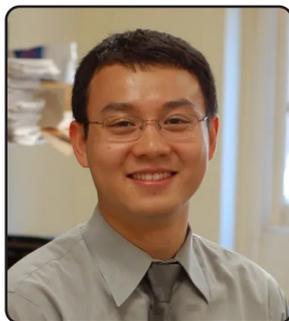
The 4th stage is how to analyze the effectiveness of policies to be launched. Each national or local government has a limited finance, and a lot of finance is required to launch policies. Thus, the best way is to launch the policies that have maximum effectiveness with minimum finance. This is for deciding policy priority to be launched among many optional policies. Two phases of policy effectiveness analysis will be presented. One is efficiency analysis of financial investment, and the other is effectiveness analysis of all policies as a whole set.

Audience Take Away:

- A conceptual framework for identifying the vulnerability to climate change.
- The methodologies to select the prior vulnerable sectors as the targets of policy formation, to set up the goal of vulnerable sector to achieve, and to mobilize the means to achieve the goal
- Governance system to be employed for establishing climate change policies based on social consensus
- A methodology of analyzing the effectiveness of climate change policies

Biography

Dr. Dai-Yeun Jeong is presently the Director of Asia Climate Change Education Center and an Emeritus Professor of Environmental Sociology at Jeju National University (South Korea). He received BA and MA Degree in Sociology from Korea University, and PhD in Environmental Sociology from University of Queensland (Australia). He was a Professor of environmental sociology at Jeju National University (South Korea) from 1981 to 2012. His past major professional activities include a Teaching Professor at University of Sheffield in UK, the President of Asia-Pacific Sociological Association, a Delegate of South Korean Government to UNFCCC and OECD Environmental Meeting, etc. He has published 13 books including Environmental Sociology, and has conducted 95 environment-related research projects funded by domestic and international organizations.

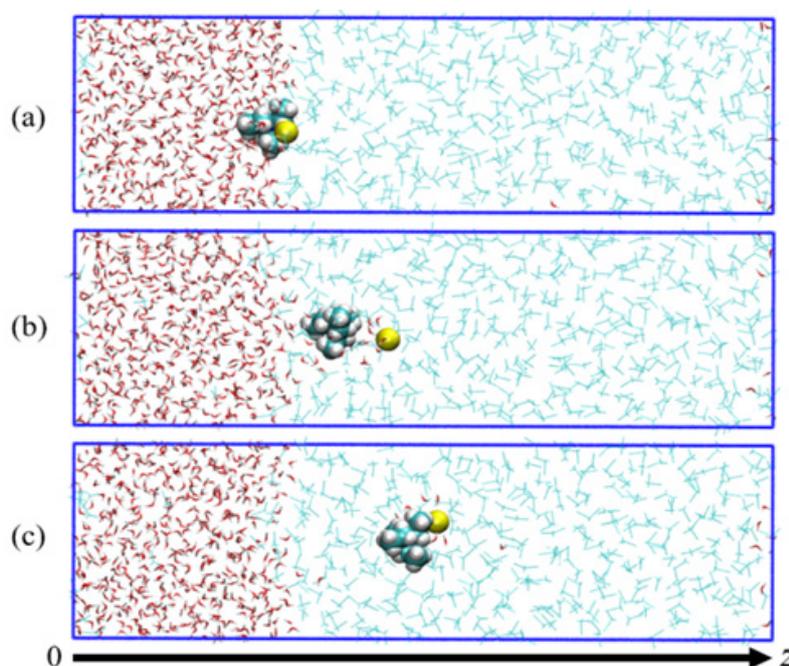


Ying-Lung Steve Tse

The Chinese University of Hong Kong, Hong Kong

Molecular dynamics simulation of phase transfer catalysis

Molecular dynamics (MD) simulations are widely used to understand different chemical and physical processes on molecular scales. The accuracy of an MD simulation depends critically on the force field, which describes the interactions between the particles and is the “heart” of an MD simulation. In this talk, I will discuss the parametrization scheme to obtain force fields for modeling phase-transfer (PT) catalysis, which is a widely exploited method of heterogeneous catalysis to enhance reaction rates in the multibillion-dollar chemical industry. While previous molecular simulation models provided our first molecular understanding of the interfaces, most force fields have been parameterized for gases or bulk liquids with no interfaces. For simulations of two immiscible fluids, the force fields should be parameterized explicitly with the interface to capture interfacial properties accurately. We obtained preliminary simulation models that are both accurate and efficient in terms of the thermodynamics of ion transfer, and they also can provide insight into how the phase transfer catalyst catalyzes the studied reactions with molecular details.



Acknowledgement: This research is supported by Research Grants Council of Hong Kong (CUHK 14300920, 14302221)

Biography

Steve Tse received his PhD in theoretical chemistry under the guidance of Prof. Hans C. Andersen at Stanford University in 2011. During his PhD work, he focused on developing new theories and simulation tools, using statistical mechanics, for studying microscopic molecular motion in stochastic models of liquids with highly cooperative dynamics. After PhD, as a Croucher Fellow at the University of Chicago, he began his postdoctoral work with Prof. Gregory Voth and Prof. Thomas Witten to study the charge transport in both aqueous solutions as well as fuel cell membranes by molecular dynamics simulations. In particular, he developed new reactive multiscale models to understand proton/hydroxide transport. In 2015 Oct, he joined the Chinese University of Hong Kong (CUHK) as Assistant Professor. Since the start of Tse research group at CUHK Chemistry Department, his team has been studying different interfacial systems including air-water and fluid-fluid/solid interfaces. A major theme of the research has been to understand the thermodynamics and the dynamics of these systems and the relationships between the two. Recently, he has started a collaboration to understand the chemical kinetics and thermodynamics of asymmetric organic reactions.

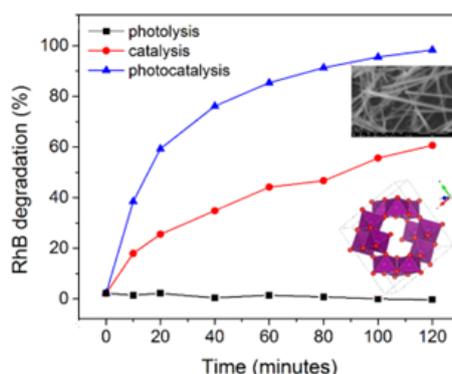
Florina Stefania Rus, Stefan Danica Novaconi, Paulina Vlazan, Madalina Ivanovici*

National Institute for Research and Development in Electrochemistry and Condensed Matter, Romania

Manganese dioxide as efficient catalyst for pollution reduction in aqueous medium

In recent decades, much effort has been made to develop nanostructures inorganic having a desired morphology, size, crystallinity and functionality. These nanostructures are widely used in applications such as electronics, materials with optical properties, energy storage and transformation, solar devices, etc. Manganese dioxide (MnO_2) is a semiconductor material that so far, has been synthesized into various polymorphic forms with different morphologies by the solvothermal/hydrothermal method presenting thermo-photo-electric activity for pollution reduction. Numerous studies have been conducted on improving the environmental purification efficiency of manganese oxides materials in order to understand key features of catalytic reaction mechanism. In this study, MnO_2 was obtained by a relatively low cost and easy hydrothermal method. The manganese oxide present nanowire morphology and alpha-phase crystallinity. The aim of this work is to prove MnO_2 application in the environmental purification systems, either as a catalyst or as a photocatalyst for the degradation of pollutants in aqueous medium. The synthesized compound was subjected to an evaluation of its catalytic activity in comparison with photocatalytic activity toward a selective degradation pathway of Rhodamine B (RhB). The experimental investigations were performed using suspensions of catalyst particles distributed in acidic RhB aqueous solution for two hours and the light irradiation for the photocatalytic study was provided by a solar simulator. The selectivity of degradation reaction was appreciated by analysing the evolution of time-dependent visible spectra of RhB and the degradation pathway was emphasized by the shift of the characteristic RhB absorbance peak toward lower wavelength values simultaneously with the formation of corresponding bands of RhB degradation by-products. Therefore, we observed a different evolution of the time-dependent visible spectra of RhB for the catalysis when compared with the photocatalysis. Enhanced results were obtained for the study carried out under solar irradiation, for which improved hypsochromic shift and higher RhB degradation percent were achieved.

Acknowledgement: This work was conducted within the National Program NUCLEU, Project Code PN 19 22 01 01, Contract No. 40N/2019 funded by Romanian Ministry of Education and Research



Audience Take Away:

- The MnO_2 act as an efficient catalyst for selective RhB degradation pathway both in dark and under solar irradiation
- The public will learn how to perform an ecological, economical photocatalytic experiment with direct environmental applications
- The difference between photolysis, catalysis and photocatalysis under friendly conditions.
- The audience will learn how to synthesize MnO_2 nanowires via low-cost hydrothermal method.

Biography

PhD student, Madalina Ivanovici studied at Industrial Chemistry and Environmental Engineering Faculty from Politehnica University of Timisoara and received bachelor and master degree in chemical engineering. Then she joined in 2018 the research group from National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara as a member team in the „Smart buildings adaptable to the climate change effects” project. Currently, her research topics are catalysis and renewable energy.



Argam Akopyan*, Raman Mnatsakanyan, Ekaterina Eseva, Polina Polikarpova, Alexander Anisimov

Lomonosov Moscow State University, Russian Federation

Highly efficient aerobic oxidative desulfurization based on tungsten carbide catalyst synthesized by the microwave method

We will present a new type of high-performance catalyst for aerobic oxidation of organosulfur compounds based on tungsten carbide. The synthesis of tungsten carbide was carried out using microwave irradiation, which makes it possible to obtain a catalyst just in 15 minutes. The synthesized catalyst was investigated by complexes of physicochemical methods: XRD, XPS, Raman, SEM, N₂ adsorption/desorption. It was shown that the key role in the activation of oxygen is played by active centers containing tungsten in the transition oxidation state (+4). The influence of the main factors influencing the conversion of dibenzothiophene was investigated. Complete oxidation of DBT can be achieved under relatively mild conditions: 120°C, 3 h, 6 bar, 0.5% wt. catalyst. The catalyst retains its activity for at least 6 oxidation/regeneration cycles. The simplicity and speed of the synthesis of the proposed catalyst in combination with its high activity and stability open broad prospects for its further use both in the process of oxidative desulfurization and for other reactions of aerobic oxidation of organic substrates.

Audience Take Away:

- The presented catalysts can be used for aerobic oxidation of various classes of compounds
- The presented results can be used by researchers in the field of the oxidative desulfurization process
- The obtained fundamental knowledge can serve as a basis for the design of a wide range of catalysts for aerobic oxidation of various substrates

Biography

Dr. Argam Akopyan studied chemistry at the Lomonosov Moscow State University, from which he graduated in 2013. In the same year he entered the postgraduate study at the Faculty of Chemistry of Moscow State University. The thesis on the topic "Oxidative desulfurization of hydrocarbons with hydrogen peroxide in the presence of transition metal salts" was defended in 2016. After defending the thesis, he continued to work on oxidative desulfurization at the Faculty of Chemistry of Moscow State University in the group of Professor A.V. Anisimov. He has published over 50 research articles in peer-reviewed scientific journals.



**Beatriz Valle*, Roberto Palos, Javier Bilbao,
Ana G. Gayubo**

University of the Basque Country, Spain

Role of zeolite properties in bio-oil deoxygenation and hydrocarbons production by catalytic cracking

The depletion of petroleum reserves and stricter environmental policies urge the search for sustainable and renewable energy sources to meet the growing global energy demand. In this scenario, lignocellulosic biomass is a renewable resource, whose valorization has attracted significant attention due to its carbon neutral lifecycle. Fast pyrolysis of biomass is a well-developed thermochemical process that produces high yield of liquid product (bio-oil), which is a complex mixture of oxygenated compounds including phenols, ketones, carboxylic acids, esters, aldehydes, alcohols, furans, and anhydrous-sugars. In comparison with catalytic hydrotreatment (HDO and hydrocracking), the catalytic cracking (CC) of bio-oil is cost-competitive in terms of process requirements since it operates at atmospheric pressure and without H_2 supply. Besides, the CC of bio-oil can be targeted towards the selective production of fuels (gasoline, diesel, jet fuel) and platform chemicals (olefins and aromatics), according to market requirements. The conversion of bio-oil oxygenates into hydrocarbons involves complex reaction pathways, such as deoxygenation (decarboxylation, decarbonylation, dehydration), cleavage of C-C bonds, oligomerization/cracking, alkylation, and hydrogen-transfer. A key factor for the successful large-scale implementation of this process is the development of selective catalysts. Zeolite-based catalysts have been widely used in the production of hydrocarbons by CC of oxygenates. Their behaviour is determined by the properties of the acid sites (Brønsted/Lewis nature, total amount and strength distribution). Pore size and structural properties are also important in regulating diffusion of reactants and products (shape selectivity), thereby affecting the selectivity to aromatics and olefins.

In this research, a comparison is established between the behavior of Y and ZSM-5 zeolites for producing hydrocarbons by catalytic cracking of bio-oil. Both zeolites have the same SiO_2/Al_2O_3 ratio (30), thereby inherent characteristics of each catalyst (microporous structure, nature of acid sites and acid strength distribution) are determined by the zeolite framework (FAU in Y zeolite, and MFI in ZSM-5). The catalysts were prepared by agglomerating each zeolite with a mesoporous $\gamma-Al_2O_3$ matrix in order to attenuate deactivation by coke deposition and improve mechanical resistance. The raw zeolites and prepared catalysts were characterized by N_2 adsorption/desorption, SEM-EDX, pyridine-FTIR, tBA-TPD, and NH_3 -TPD techniques. The experiments were carried out in a continuous two-step catalytic cracking system (TS-CC) at 450 °C. Both catalysts are highly selective to C_5 - C_{12} hydrocarbons, with a composition strongly affected by the porous structure and acidity of the zeolite. The HZSM-5 catalyst (high acid strength and Brønsted/Lewis ratio) promotes cracking and deoxygenation reactions that lead to C_2 - C_4 olefins which condensate into aromatics, yielding 9% of 1-ring aromatics (3% BTX) and 4% of naphthalenes for a feed conversion of 85 %. These reactions are less favored over the HY catalyst (with large cavities located between the straight micropores), which promotes olefins oligomerization and hydrogen-transfer reactions, yielding 14% of highly aliphatic gasoline (> 30% linear paraffins) and 5% of C_{13} - C_{20} diesel fraction (> 90% long chain paraffins). The remaining upgraded bio-oil obtained with both catalysts is composed of light oxygenates, with ketones, acids and esters as main components and low concentration of phenolic compounds.

Audience Take Away:

- It addresses the valorization of real raw bio-oil, scarcely studied in the literature
- Conversion of stabilized bio-oil feedstock (with 20 wt% of methanol) is studied so that the findings would be applicable to the scaling-up of the process.
- Two original strategies that address the catalyst particle design (agglomeration of zeolite), and the reaction system (two-step catalytic cracking reactor) have been combined.

- Detailed composition of oxygenated liquid product is reported, which is essential for assessing its potential for further valorization (integral valorization of CC products)
- Provide new and wide information of raw bio-oil cracking through a comparative study of the behavior of two zeolites with similar total acidity but different framework.

Biography

Dr. Valle received her PhD degree with honours in Chemical Engineering in 2008 at the University of the Basque Country (Spain). She is currently research fellow at the Catalytic Processes and Waste Valorization group (CPWV) of the Chemical Engineering Department at the same institution. Her research lines focus on heterogeneous catalysis, reaction mechanism/kinetics, valorization of biomass derived oxygenates and pyrolysis oil into H₂, fuels and value-added chemicals. She has directed two Doctoral Theses, published 57 research articles in international peer reviewed journals (39 Q1, 20 first author, h-index 28) with more than 2470 total citations. She is co-author of 105 contributions (45 oral and 60 poster) in national and international conferences.



Orlando Elguera

University of São Paulo, Brazil

Review of research topics for scaling-up of sonochemical reactors (sono-reactors)

This study is aimed to review the topics of chemical engineering to take in consideration for the scaling-up of reactors, in order to perform processes based on the application of the sonochemistry at industrial level. Sonochemistry is an emergent technology, defined as chemistry made with ultrasound. The characteristic ultrasound frequencies are in the range of 1-10MHz, and in particular for sonochemistry in the sub-range 16-100 KHz. Chemical effects of ultrasound exist when there are changes in the path-ways of reactions, yields and/or selectivities of the products due to the ultrasonic activation. At laboratory level, the sonochemistry has shown fantastic results, because it is based on the phenomenon of acoustic cavitation in liquids, thus, producing very high temperatures (some thousands of Kelvin degrees) and high pressures (some hundreds of atmospheres) during very short times (from tenths to hundreds of microseconds). Cavitation is the phenomenon with the most important effect for intensification of physical and chemical processing. Under these conditions, the yields of sonochemical reactions increase drastically, and their selectivities are improved, thus generating new mechanisms of reaction involving inorganic and organic syntheses. It is not easy to reproduce experimental results of quantification of sonochemical intensity, which is significant for the efficient scaling-up of sonochemical reactors (sono-reactors) for the progress of industrial applications of sonochemistry. This technology has application at industrial level for the treatment of waste-water and black-water. Sonochemistry can be considered as Green Chemistry, presenting the following advantages: low waste, low consumption of materials and energy with optimized use of non-renewable resources and use of renewable energies. Few studies were aimed about optimum design and scaling-up of sonochemical reactors. The implementation of sonochemistry at the industrial level will be feasible when the use of cavitation energy can be adequately controlled.

Biography

Orlando Armando Elguera Ysnaga is from Peru. He completed his Major in Chemical Engineering from the National University of Engineering, Lima-Peru, and also Bachelor of Science with a Major in Chemical Engineering from the National University of Engineering, Lima-Peru. Studied for Master of Science with Major in Chemistry from National University of Engineering, Lima-Peru. He did Doctor of Science with Major in Analytical and Inorganic Chemistry from University of São Paulo, São Paulo-Brazil. Now he is working as an Independent Consultant in Environmental Matters of Mining and Sustainable Development and has joined as editorial board member for International Journal of Forensic and Medical Jurisprudence.



Fernanda A. Siqueira*, Luiz S. Longo, Jr, Renata C. Z. Mendonça, José Carlos Q. Arêas, Matheus Boaretto, Larissa M. Silva, Livia Y. Sawada

Federal University of Sao Paulo, Brazil

Dynamic kinetic resolution of primary benzylamines by using recyclable palladium supported on dolomite

Enantiomerically pure amines are important building blocks for the synthesis of molecules with potential biological activity and are employed as essential intermediary to chemistry, pharmaceuticals and agrochemistry industries. Dynamic Kinetic Resolution (DKR) has been a method largely employed to synthesize optically pure compounds, in which both Kinect enzymatic resolution and racemization steps should demonstrate great compatibility. In this work, palladium catalyst supported on dolomite (2.5% PdDOL) had both activity and selectivity studied in DKR reactions of different benzylamines, which are substituted at the aromatic ring with methyl and fluorine groups. Several reaction conditions were used in the catalytic activity studies of the 2.5% PdDOL, including the use of different temperatures (80 °C and 95°C), reaction times (6 to 24h) and acylating agents (ethyl acetate, isopropyl acetate and isoamyl acetate). Furthermore, the effects of four different ionic liquids, two ammonium salts and two phosphonium salts, as additives was also investigated.

For the first time in literature a palladium catalyst supported on dolomite was used for Dynamic Kinetic Resolution reactions of primary amines. The results obtained demonstrated good activity and selectivity, since the starting material was converted to the desired product by up to 100%. The temperature of 95 °C provided excellent conversion values for (*R,S*)-1-phenylethylamine, that was used as a model compound. Ethyl acetate as acyl donor proved to be the most efficient acylating agent, as it presents a smaller and less hindered chain, facilitating the enzymatic acetylation step. Reaction times were optimized using ionic liquids, especially for (*R,S*)-1-phenylethylamine and (*R,S*)-1-(4-fluoro)phenylethylamine.

Audience Take Away:

- The audience will be able to show the perspectives about the use of catalysis in amines synthesis;
- The audience will help to improve the disclosure of results and international network

Biography

Dr. Fernanda A. de Siqueira is a Professor of Chemistry at Federal University of São Paulo, Brazil. She obtained her undergraduate degree in Chemistry (2001) from Federal University of Juiz de Fora, Minas Gerais, Brazil. Siqueira received her Ph.D. in Chemistry from the University of São Paulo in 2008. After 2 years as a postdoctoral fellow at University of Campinas, she was appointed to the Department of Chemistry at Federal University of São Paulo as a Lecturer. She was promoted to Associate Professor in 2018. Current research in the Siqueira's Lab emphasize the metal heterogeneous catalysis and dynamic kinetic resolution.



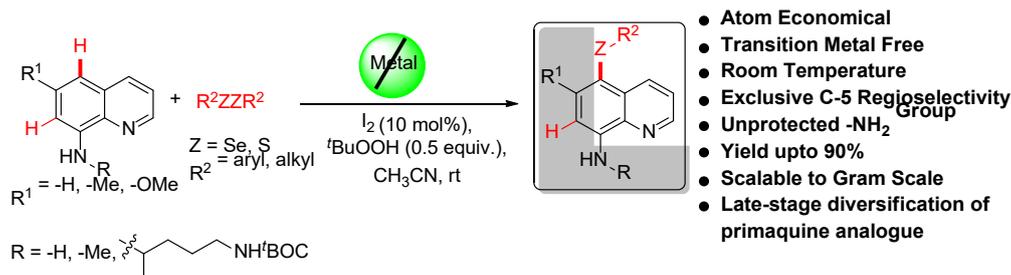
Vipin Kumar, Devalina Ray* and Biswajit Saha

Amity University, India

Regioselective and atom economical metal free C-5 chalcogenation of 8-aminoquinolines under mild conditions

A novel and simple transition metal-free protocol for expedient C-H functionalization leading exclusively to the regioselective generation of C-5 chalcogenated 8-aminoquinoline analogues in up to 90% yield at room temperature (25 °C) has been demonstrated. This methodology is a direct and eco-friendly approach to the atom-economical utilization of diaryl/dialkyl chalcogenides for highly efficient access to chalcogenated quinolines and is scalable to the gram scale without significant decrease in the yield of the product. It represents a practical alternative to all other existing metal-catalyzed functionalization of 8-aminoquinoline derivatives with broad functional group tolerance. The successful implementation of this protocol is reflected through the conversion of diversified group of 24 substrates to respective regioselective C-5 chalcogenated products in good to excellent yields. The reaction was found equally efficient in gram scale and no significant reduction in the yield was observed. The controlled experiments based on radical quenching with 2,2,6,6-Tetramethylpiperidine 1-oxyl (TEMPO) and butylated hydroxytoluene (BHT) couldn't reduce the yield of product while no additional compound was determined in the reaction mixture. Furthermore, no difference was detected in the rate of reaction during the study of kinetic isotope effect which reveals that the cleavage of C5-H bond is not involved in rate determining step. Both observations collectively indicates that the reaction possibly proceeds through an ionic S_NAr reaction pathway at room temperature.

Furthermore, the potentiality for the functionalization of free amines in chalcogenated-8-aminoquinolines provides an attractive perspective for further elaboration of the amine substituent through chemical manipulations. The applicability of the standardized method has been augmented through late-stage antimalarial drug derivatization of primaquine analogues.



Audience Take Away:

- The presentation will provide a broad scope for transition metal free catalysis toward the C-H bond functionalization and its application in various class of substrates and drug precursors. It opens up a new avenue for greener approach to the existing protocols and provides an effective alternative to the transition metal catalyzed reactions.
- The research work demonstrated can be considered as the advanced version of the basic teaching on heterocyclic compounds and their reactions. The existing contents can be expanded and more informations can be gained from the experimental results which will be cited through the presentation. This research can obviously complement and contribute to expand and the existing research and teaching of faculties. The developed method has the potential to provide practical solution to many regioselective synthesis and functionalization of heterocyclic compounds.

Biography

Dr. Devalina Ray is currently employed as Assistant Professor in the Department of Biotechnology, Amity University, Noida, UP, India. She pursued B.Sc(H) in Chemistry followed by M. Sc in Organic Chemistry from Kalyani University, WB, India. In 2008 she received Ph.D. in chemistry from IIT-Kharagpur, India. She was a postdoctoral researcher at the University of Texas Medical Branch, and University of Nebraska Medical Centre, USA, followed by Myongji University and Hanyang University, South Korea. Thereafter, she joined Department of Chemistry, IIT- Delhi as research associate and young scientist. Her research interests involve synthetic organic chemistry, green chemistry, medicinal and natural product chemistry.



Ashanendu Mandal

University of Calcutta, India

Removal of toxic phenol from wastewater using low-cost adsorbents

Phenol being toxic in nature needs to be removed from wastewater before its surface discharge. This research aims for removal of phenol using four biological waste adsorbents guava tree bark, rice husk, neem leaves, activated carbon from coconut coir and four industrial waste adsorbents rice husk ash, red mud, clarified sludge from basic oxygen furnace, activated alumina. The surface characterization of adsorbents were carried out by SEM, XRD, FTIR and BET analyzers. The phenol removal percentage were investigated with the variation of initial phenol concentration (5-500 mg/L), initial pH (2-12), adsorbent dose (0.10-20 gm/L), temperature (25-50°C) and contact time (30-600 min). The maximum removal was obtained as high as 97.50%. The experimental results were used for kinetic, isotherm and thermodynamic studies. The kinetic analysis showed that the pseudo-second order was best fitted for all adsorbents except red mud and the adsorption mechanism was supportive of film diffusion, intra-particle diffusion and chemisorption for all adsorbents. The isotherm analysis suggested that Freundlich isotherm model was best supportive for guava tree bark, rice husk, neem leaves, activated carbon, red mud and activated alumina, whereas Langmuir and D-R isotherm was best supportive for rice husk ash and clarified sludge respectively. The thermodynamics study showed that the adsorption processes were spontaneous, random and endothermic or exothermic in nature. The phenol removal efficiencies with real industrial wastewater collected from a coke oven plant were also studied in this research work. Further the scale-up design, safe disposal and regeneration of adsorbents were carried out to examine their commercial applications. The innovative ANN modeling was also studied which showed that the experimental and predictive data were within allowable range. The research finally reveals that all the adsorbents are substantially effective for phenol removal and can therefore be considered for circular economy.

Biography

Ashanendu Mandal has worked in ONGC for more than 34 years in offshore and onshore oilfields. He is graduated as B. Sc (Chemistry) and B. Tech (Chemical Engineering) from University of Calcutta and post-graduated as M. Tech in Chemical Engineering from IIT, Kharagpur and MBA in Finance from IGNOU, New Delhi. He is the lifetime professional member of Indian Chemical Society and Indian Science Congress. He is now doing research in University of Calcutta. He has been recognized with the Best Researcher Award 2020 by VD Good International Professional Association. He has participated in many international conferences in more than 17 countries as invited speaker, panelist, roundtable moderator and session chairman.



Manas Ranjan Senapati

Trident Academy of Technology, India

Nanocatalysis in biofuels- an overview

The concept of biofuel was introduced in 1885 when Dr. Rudolf Diesel built the first diesel engine with the intention of running it on vegetative origin. He displayed his engine for the first time at the Paris show of 1900 and astounded everyone when he ran the patented engine on any hydrocarbon fuel available, which included gasoline and peanut oil. In 1912 he stated, "The use of vegetable oils for engine fuels may seem insignificant today. With increasing demand of petroleum products throughout the world and its depleting resources has now encouraged the scientists and research workers to find the alternative to diesel particularly for transportation sector. Biodiesel can be extracted from vegetable oil and one such renewable alternative is *Jatropha Curcas*. Catalysis plays an important role in transesterification of vegetable oils. Nano particles are being used in biological catalysis augmenting the process of transesterification. Many aspects production base oil resources, their physical properties, transesterification and effects of catalysts on the process, stability and Iodine value of the various oils, advantages of biodiesel vis-à-vis diesel and future prospects of the system have been discussed in this paper.

Biography

Dr. Manas Ranjan Senapati (b.1968) is working at present as Professor and HoD of Chemistry in Trident Academy of Technology, Bhubaneswar. He is nominated as Dean Computer Application & Science of Biju Patnaik University of Technology, Odisha. He earned his doctoral degree from Utkal University, Bhubaneswar in 1993 and also did his post doctoral research as CSIR Research Associate. His areas of interest include solute-solvent interaction, solid waste management, pollution control, climatology, green & sustainable Chemistry and biofuels. He has published more than thirty five research papers in national and international journals of repute.

Participants List

Thomas J. J. Müller Heinrich-Heine-Universität Dusseldorf, Germany	7
V. Beschkov Bulgarian Academy of Sciences, Bulgaria	8
Edward Lee-Ruff York University, Canada	9
Yuto Nakano National Institute of Technology, Oyama College, Japan	11
Yakha Vissurkhanova E. A. Buketov Karaganda University, Kazakhstan	12
Anna M. Kisiela-Czajka Wroclaw University of Science and Technology, Poland	13
Demirov A.P National University of Science and Technology MISIS, Russian Federation	15
Shabanova Chimnaz Mamed Azerbaijan National Academy of Science, Azerbaijan	16
Md Nurul Islam Siddique University Malaysia Terengganu, Malaysia	19
Víctor Cerda University of the Balearic Island, Spain	21
Andrea Czompa Semmelweis University, Hungary	22
Bruno Mattia Bizzarri University of Tuscia, Italy	23
Mohamed Ezeldin Osman Peoples' Friendship University of Russia, Russia	24
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Mridusmita Barooah National Institute of Technology, India	28
Rabeharitsara Andry Tahina Polytechnic Engineer School of Antananarivo University, Madagascar	29
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Alexander G. Ramm Kansas State University, United States	34
Anne M. Gaffney University of South Carolina, Columbia, South Carolina, USA	35
L. Kollar University of Pecs, Hungary	36
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Madalina Ivanovici National Institute for Research and Development in Electrochemistry and Condensed Matter, Romania	40
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