



CATALYSIS WEBINAR
BOOK OF ABSTARCTS



SCHOLARS INTERNATIONAL WEBINAR ON:

CATALYSIS AND CHEMICAL SCIENCE

THEME: "THE ROLE OF NEW TECHNOLOGIES IN THE FIELDS OF CATALYSIS AND CHEMICAL SCIENCE"

24-25
MAR 2021
WEBINAR

<https://scholarsconferences.com/catalysis-webinar/>

SCIENTIFIC PROGRAM

DAY 1 | 24 MARCH | Wednesday

11:00-17:00 (GMT)

11:00-11:10 Introduction

KEYNOTE FORUM



11:10-11:50

Title: Concepts of surface tension and adsorption revisited

Abraham Marmur, Technion - Israel Institute of Technology, Israel

13:10-11:30 (Speaker Local Time)



11:50-12:30

Title: Development of Industrial Catalysts Path to Commercial Applications

Erick D Gamas, The Business Shop-Chemical Engineering Services, United States

06:50-07:30 (Speaker Local Time)



12:30-13:10

Title: The Key Role of Catalysts and Adsorbents in Energy Transition

Meritxell Vila, MERYT Catalysts & Innovation, Spain

13:30-14:10 (Speaker Local Time)

13:10-13:30 - REFRESHMENTS BREAK



13:30-14:10

Title: Double-Duty Complexes: Catalysis and Biological Activity in One Neat Package

Joseph Merola, Virginia Polytechnic Institute and State University, USA

09:30-10:10 (Speaker Local Time)

SCIENTIFIC SESSION



14:10-14:40

Title: Understanding the effect of chemical reactions on the surface grain structures: Tube failures in Economizers

Ravi Kiran Kaipa, Northumbria University, UK

19:40-20:10 (Speaker Local Time)



14:40-15:10

Title: Catalytic combustion in reverse flow reactor with integrated adsorption

Javier Fernandez, University College London, UK

14:40-15:10 (Speaker Local Time)



15:10-15:40

Title: Tuning the Electronic Structure of Ag-Pd Alloys to Enhance Performance for Alkaline Oxygen Reduction

José Zamora Zeledón, Stanford University, USA

08:10-08:40 (Speaker Local Time)

SCIENTIFIC PROGRAM

15:40-16:00 - REFRESHMENTS BREAK



16:00-16:30

Title: Algorithmic Signalling Controlling Enzymatic Catalysis with Artificial Intelligence Robotic Approach

Ozan Emre EYUPOĞLU, Istanbul Medipol University, Turkey

19:00-19:30 (Speaker Local Time)

16:30-17:00 - B2B MEETINGS AND NETWORKING

DAY 2 | 25 MARCH | Thursday

11:00-17:00 (GMT)

11:00-11:10 Introduction

KEYNOTE FORUM



11:00-11:40

Title: Green Chemistry in the Generic Pharmaceutical Industry

Apurba Bhattacharya, Texas A&M University, USA

06:00-06:40 (Speaker Local Time)



11:40-12:20

Title: Catalytic processes under continuous flow- Current trends and applications

Manuel Nuno, Vapourtec Ltd., UK

11:40-12:20 (Speaker Local Time)

SCIENTIFIC SESSION



12:20-12:50

Title: Light-Activated Quantum Dot Potentiation of Antibiotics to Treat Drug-Resistant Biofilms

Dana Stamo, University of Colorado Boulder, USA

06:20-06:50 (Speaker Local Time)



12:50-13:20

Title: A New Approach for Modeling of Catalytic Processes in Industrial Column Apparatuses

Christo Boyadjiev, Bulgarian Academy of Sciences, Bulgaria

14:50-15:20 (Speaker Local Time)

13:20-13:40 - REFRESHMENTS BREAK

SCIENTIFIC PROGRAM



13:40-14:10

Title: Controlled graphite functionalization by photocatalytic oxidation for rationally engineered electrocatalysis

Niels Ostyn, KU Leuven, Belgium

14:40-15:10 (Speaker Local Time)



14:10-14:40

Title: Microbial-based Bioremediation of an Exemplar Organophosphorus Chemical Warfare Agent

Alaa Hassan Al-Farttoosy, University of Basrah, Iraq

17:10-16:70 (Speaker Local Time)



14:40-15:10

Title: Reaction Kinetics in Chemical Engineering

Christo Boyadjiev, Bulgarian Academy of Sciences, Bulgaria

16:40-17:10 (Speaker Local Time)

15:10-16:00 - Networking and B2B Meetings

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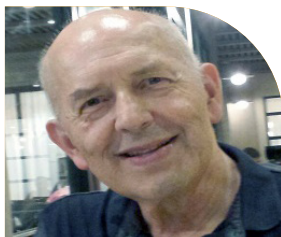
**KEYNOTE
SPEAKERS**

Day 1



CATALYSIS WEBINAR

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Abraham Marmur

Technion – Israel Institute of Technology, Haifa, Israel.

Biography

Abraham (Avi) Marmur received his D.Sc. in 1974 at the chemical engineering department, Technion – Israel Institute of Technology, then spent two years in Buffalo, NY as a postdoc with Eli Ruckenstein. He returned to Technion in 1976 as a faculty member and is now a Professor Emeritus. He spent two Sabbatical years, one at the University of Wisconsin, Madison, and another at the IBM Almaden Research Center. Prof. Marmur has worked and published extensively in the field of interfacial phenomena, and his publications are highly cited. In addition, he was an editor of Reviews in Chemical Engineering, and was on the advisory committee/editorial board of Journal of Colloid and Interface Science, Journal of Adhesion Science and Technology, Advances in Colloid and Interface Science, Colloids and surfaces A, Surface Reports, Entropy, and Surface Innovations. At Technion, professor Marmur received awards for excellence in research and in teaching.

Concepts of surface tension and adsorption revisited

The fundamental concepts of surface tension and adsorption are revisited. It is shown that surface tension of a liquid can be defined without the concept of dividing surface and that this definition also clarifies the adsorption equation. In addition, it is demonstrated that very negative pressures must exist in the interfacial layer. Finally, the concept of surface tension of a solid is critically discussed.



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Erick D Gamas

The Business Shop-Chemical Engineering Services, USA

Biography

Erick D Gamas completed his B.Sc. in Chemical Engineering from Metropolitan University of Mexico, M.Sc. in Applied Mathematics to Chemical Engineering from Metropolitan University of Mexico, Ph.D. in Chemical Engineering from the University of Houston, USA. He has overall 37 years of experience in Chemical Engineering applications to Heterogeneous Catalysis R&D, Development of industrial catalysts and Process Development of Catalytic Processes. He got collaborated with major Research and Engineering companies

- Mexican Institute of Petroleum
- ExxonMobil Research and Engineering
- UOP (Honeywell)
- Albemarle Catalysts
- Clariant Catalysts

He also got 12 technical papers and five US patents granted on his name.

Development of Industrial Catalysts Path to Commercial Applications

Most of the materials that sustain modern life in industrialized economies involve a series of interconnected heterogeneous catalytic processes in their transformation of raw materials to consumer goods. From production of fertilizers that sustain food production, the production of transportation and heating fuels and basic chemicals in oil refineries, the transformation of basic petrochemicals to consumer goods, to the processes that control emission of contaminants to the environment, the complete production network is supported by a multitude of catalytic materials enabling economically feasible manufacturing processes with high levels of safety in their operations. The global market for industrial catalysts had an estimated value, as of 2019, at ~34 billion (3.9 x 10⁹) USD and had a compound annual growth rate of 4.4% from 2020 to 2027. These estimates have, however, been strongly affected by the 2020 global pandemic shifting markets from production of fuels to much higher production of basic

petrochemicals to manufacture plastics. The demand for catalysts for treating fuels will decrease and will shift to a much higher demand for catalysts involved in the production of petrochemicals.

The detailed understanding on how solid catalysts enable otherwise impossible or uneconomical chemical reactions is abundant. Development of complex analytical techniques has allowed the understanding of why and how many materials work at the molecular level. Much is understood at the microscales level, such is not the case of the macro scale production and manufacturing of solid catalysts. Even less is available as public information as the information might represent a competitive advantage for the process owner. From the initial conception of a new material, or a new shape of a known material, the process engineering concepts that determine the shape of solids, the sourcing of raw materials and the manufacturing of catalysts, the sales and procurement of commercially proven materials to the start-up/shutdown, monitoring and troubleshooting of catalytic processes. An analysis of the complex path to commercialization of solid catalysts will be presented.

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Meritxell Vila

MERYT Catalysts & Innovation, Spain

Biography

Dr. Meritxell Vila completed her PhD in Chemistry (Chemical Engineering) from the University of Barcelona. I started my professional life working for REPSOL at the Research Centre in Cartagena (Spain) studying Ion Exchange Resin catalysts for the ETBE/MTBE synthesis. After spending several years on Process Development, at the pilot plant units of the Research center, related with gasoil hydrotreatment and gasoline hydrodesulfurization, I moved to the Repsol Cartagena refinery to work at the Quality Control Laboratory and the Process Department in the Lubricants and Hydrotreatment divisions. I was responsible for Solomon studies and Industrial trials for innovative processes and the Catalysts Coordinator of the refinery.

In 2011, I joined IMCD Spain, moving into chemicals distribution, where I have been working as Product and Project Manager representing the major international catalyst and adsorbent manufacturers in the Spanish and Portuguese markets.

In February 2016, I have started my own company MERYT Catalysts & Innovation to offer my knowledge and expertise both to customers and suppliers and help to grow their respective businesses.

The Key Role of Catalysts and Adsorbents in Energy Transition

We are experiencing an unprecedented change in the way we supply energy. Climate change has led us to reduce CO₂ emissions, which means a complete change in our traditional way of manufacturing fuels and chemicals. Catalysts and Adsorbents have always helped us in the processes of obtaining fuels and chemical products. And now they will also continue to do so, facing the new challenges of: Crude Oil To Chemicals (COTC) refinery, New Biofuels and Green Hydrogen. In this conference, we will see in detail how Catalysts and Adsorbents continue to be our best friends in these great challenges that await us.

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Joseph S. Merola

Virginia Tech, Blacksburg, USA

Biography

Joseph S. Merola is a Professor of Chemistry at Virginia Tech and a graduate of Carnegie-Mellon University (B.S. Chemistry, 1974). He received his Ph.D. in chemistry in 1978 from M.I.T under the direction of Professor Dietmar Seyferth. In 1978, he joined the Corporate Research Laboratories of Exxon Research and Engineering Co in New Jersey. In 1987, he joined Virginia Tech where he has been ever since, although he has held many different roles over his time there. Professor Merola is a Fellow of the American Chemical Society and a Fellow of the American Association for the Advancement of Science. He has published over 120 papers in the organometallic chemistry and catalysis field.

Double-Duty Complexes: Catalysis and Biological Activity in One Neat Package

"Piano-Stool" complexes of transition metals have been known since the beginning of "modern" organometallic chemistry, often dated to the serendipitous discovery of ferrocene in 1951. Since then, the number of pi-complexes of metals including other sandwich and half-sandwich compounds (piano-stools) is difficult to quantify. A "Google Scholar" search on the terms "piano-stool" or "half-sandwich" complexes returned over 150,000 hits and that is probably not a complete accounting. With at least that number in the literature, is there anything new to add to the field? It is the hope that this lecture will convince you that the answer is "yes!"

This talk will describe chemistry of rhodium and iridium piano-stool complexes for:

- A. Hydrogenation/dehydrogenation chemistry
- B. Anti-microbial activity including anti-TB and anti-MRSA compounds.
 1. A tantalizing look at new anti-viral activity

In both areas, how changing the piano-stool metal, pi-ligand, and other ligands can tune both catalytic activity and biological activity will be discussed.

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**SCIENTIFIC
TRACKS
&
ABSTRACTS**
Day 1



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Ravi Kiran Kaipa

Northumbria University, United Kingdom

Biography

I am Ravi Kiran Kaipa, a recent master's degree graduate in Mechanical Engineering from Northumbria University with an immense interest in the Aerodynamics and a contentious and diligent professional. I've worked on some of the projects which deals with the batteries in the electric go-kart and the reactions that are caused on the economizer tubes which ultimately causes its failure for the undergraduate project which gives me some knowledge based on the research conducted in these regards.

Understanding the effect of chemical reactions on the surface grain structures: Tube failures in Economizers

A research based on an extensive study conducted on the Failure in the Tubes of the Economizers in a thermal power station for its grain structures and analysing the different kinds of failed structures by calculation of absolute reaction rates is formulated in terms of quantities which are available from the potential surfaces which can be constructed at the present time. The probability of this state is calculated using ordinary statistical mechanics. This probability multiplied by the rate of decomposition at the grain surface level gives the specific rate of reaction. The occurrence of quantised vibrations in the reacted space leads to relative reaction rates for isotopes quite different from the rates predicted using simple kinetic theory. The necessary conditions for the general statistical treatment to reduce to the usual kinetic treatment are given.

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Javier Fernandez

University College London, UK

Biography

Javier Fernández obtained his bachelor degree in Chemical Engineering in 2007 and his masters degree in Environmental and Processes Engineering in 2010 from the University of Oviedo, Spain, while he worked in research activities for different companies such as Saint-Gobain, Biogas Fuel Cell and XSTRATA. In 2011 he started his PhD in Chemical Engineering, working in the LOWCARB ERC Project. He received the Cum Laude award in 2014 and then he moved to the Warwick Manufacturing Group, where he worked as a research fellow. He also worked in a spin-out company (Stoli Catalysts Ltd) for a year. In 2017, he was appointed as Assistant Professor in Chemical Engineering and finally as lecturer in Chemical Engineering in 2020 at University College London.

Catalytic combustion in reverse flow reactor with integrated adsorption

High flow rate methane-containing emissions (0.1-0.6 %) are released during coal mine operation (ventilation gases). In the last years, the concern about these emissions has increased; since methane is an important greenhouse effect gas (its global warming potential is 23 times higher than the one for CO₂). Hence, its contribution to the environmental impact in the coal mining has been determined taking into account the carbon and ecological footprints.

Considering the emission flow rates and methane concentration, catalytic combustion could be an interesting alternative for the treatment of these emissions. Therefore, the use of a regenerative system integrated in the reactor (reverse flow reactor, RFR), which is based on the use of regenerative beds for heating the feed and in the change of flow direction, leads to a high energetic efficiency and to autothermal operation (the heat from the reaction is used to heat the feed stream, without needing external energy).

The RFR operation has been experimentally studied by using a pilot scale reactor (0.05 m diameter and 0.4 m bed length). Taking into account that the ventilation air has no sulphur compounds, the most suitable catalyst for methane combustion is palladium. Therefore, a monolithic catalyst (Pd/Cordierite) has been chosen, because this kind of beds has key advantages, such as a lower pressure drop, but also some drawbacks, as a reduction in the reactor stability.

Firstly, the intrinsic kinetics for the methane combustion has been determined, first-order dependence on methane concentration providing the best fitting to the experimental data. Then, considering that several coal mines present high CO₂ concentrations (up to 2.5 %), its possible effect on the kinetics has been analyzed, determining that this effect is negligible. On the other hand, mine ventilation systems present high moisture contents (water molar fraction between 0.02 and 0.05), water being considered a strong inhibitor in catalytic combustion. This behavior has been modeled considering a Langmuir-Hinshelwood approach.

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Concerning to the operation with the reverse flow reactor for the catalytic combustion of the coal mining ventilation air, firstly the influence on the reactor performance of the switching time (50 – 600 s), the initial methane concentration (1000 – 6000 ppm) and the flow rate (15 – 30 NL/min) was studied, concluding that switching time and initial methane concentration are key the parameters in order to avoid the extinction of the reactor.

The moisture inhibition effect has been also considered in the operation of the reverse flow reactor. Therefore, it was observed that it has an important influence on the reactor stability, given that an increase in the methane initial concentration was needed in order to keep reactor stability at a given switching time in presence of H₂O. In order to overcome this problem, a new approach is taken in this PhD, consisting of adding an adsorbent bed at both ends of the catalytic zone. An appropriate selection of the adsorbent (-Al₂O₃) leads to a totally compensation of the effect of the moisture in the reactor performance.

The information from the experiments allows the validation of a dynamic one-dimensional heterogeneous model for the RFR, which was solved using a MATLAB code. Using the experimentally validated model, and considering a typical coal shaft of the Asturian basin (Candín) with a flow rate of 45 m³/s and a methane concentration of 3000 ppm, the influence of the humidity, concentration and flow rate variations in the performance of a full-scale reverse flow reactor was analyzed.

What will the audience take away from your presentation? (Try to list 3-5 specific items)

- Explain how the audience will be able to use what they learn? This presentation could boost collaborations as people would like to study the feasibility of this innovative reverse flow reactor. They will learn how temperature could be controlled with this approach, so this could be a breakthrough in reaction engineering.
- How will this help the audience in their job? This presentation will show a possible new technology for combustion and exothermic reactions. This temperature control is a new approach which could mean new research lines for other exothermic reactions.
- Is this research that other faculty could use to expand their research or teaching? Possible academics and industries could be interested in testing their catalysts with this approach. Strong collaborations could be developed and discussed.
- Does this provide a practical solution to a problem that could simplify or make a designer's job more efficient? This can have an impact on thermal or catalytic combustion or high temperature processes.
- Will it improve the accuracy of a design, or provide new information to assist in a design problem? It will provide a much wider variety and possibilities for desired products in catalytic reactions.

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José A Zamora Zeledón

Stanford University, USA

Biography

PhD Candidate J. A. Zamora Zeledón advances the discovery and fundamental understanding of material-property-relationships of electrocatalysts with applications for renewable electrochemical-energy technologies. The objective of his studies is to employ combined systematic experimental and physics-based modeling methods to fundamentally understand the nature and properties of electrocatalyst active sites to tune performance for heterogeneous electrochemical reactions such as oxygen reduction. He uses the Stanford Nano Shared Facilities and the Stanford Synchrotron Radiation Lightsource for in-depth material characterization. To evaluate the activity of well-controlled thin-film catalysts he employs various electrochemical techniques to analyze the relationships between current, overpotential, time, and material stability.

He collaborates with the Nørskov Group at the Technical University of Denmark to perform supporting representative DFT modeling. He is a Gates Graduate Fellow. He worked with Prof. Alex Bell at UC Berkeley during his undergraduate studies and was selected as a Chevron scholar for his contributions to energy research.

Tuning the Electronic Structure of Ag-Pd Alloys to Enhance Performance for Alkaline Oxygen Reduction

The large overpotential needed for the oxygen reduction reaction (ORR) is a factor limiting the large-scale deployment of clean energy technologies such as fuel cells (FCs) and metal-air batteries. Designing strategies to enhance catalyst performance for the ORR is one method towards enhancing these technologies. Focusing on H₂ FCs, anion exchange membrane FCs are an attractive alternative to proton exchange membrane FCs because some theoretically active, yet acid-unstable, catalysts, such as Ag, can be stabilized in alkaline media. Ag-rich catalysts are specifically ideal because of their low cost and abundance compared to other catalysts materials (e.g. Pt). Better understanding the nature of intrinsic enhancements for the ORR on alloys will help in the development of new ORR alloy electrocatalysts.

One strategy to enhance ORR activity is to alloy Ag, which binds oxygen-adsorbates too weakly, to a metal such as Pd, which binds them too strongly and is also very active. In this work, we use a thin-film model system to show intrinsic activity enhancements for the ORR on Ag-Pd catalysts, resulting in activities higher than those of both parent materials even after decreasing the Pd content by half. Physical characterization indicates that the films alloyed, are flat/smooth, and have modified electronic structures. ORR evaluation via cyclic voltammetry in 0.1 M KOH indicates the films with +40 at% Pd have activities, at 0.9 V vs. RHE, greater than the linear combination of pure Ag and Pd activities. Ag_{0.1}Pd_{0.9} is the most enhanced thin-film alloy demonstrating a 5-fold activity enhancement relative to pure Pd. By correlating density functional theory with experimental measurements, we propose that Ag is modifying Pd's surface electronic structure by weakening oxygen-adsorbate binding mainly via ligand effects. These enhanced Ag-Pd ORR catalysts could facilitate the large-scale implementation of efficient clean energy electrochemical systems.



Ozan Emre EYUPOGLU

Istanbul Medipol University, Turkey

Biography

Dr. Ozan Emre Eyupoglu is an Assistant Professor in School of Pharmacy at Istanbul Medipol University, Istanbul, Turkey. He received his PhD Degree from Graduate School of Natural & Applied Sciences, Chemistry (Biochemistry), Karadeniz Technical University, Turkey in 2017. His area of interest includes Health Sciences, Medicine, Basic Medical Sciences, Biochemistry, Biophysics, Biomolecules, Proteomics and Biological Spectroscopy. He has published number of researches and conference articles about the chromatographic analysis and antioxidant activities of medicinal plants in reputed journals. He is closely related to topics such as artificial intelligence, machine learning, and innovative techniques, and plans studies for processing biochemical data for disease diagnosis. He is an interdisciplinary scientist who specializes in developing on-line chromatographic methods. He supervised 2 Master degree candidates who are making thesis on the coagulation system and aromatherapy recently.

Algorithmic Signalling Controlling Enzymatic Catalysis with Artificial Intelligence Robotic Approach

Bioregulation can be controlled by monitoring the frequency of the 3x3 matrix code produced by artificial intelligence with an algorithm that combines the state-of-the-art learning algorithm with the enzyme pathway signalling mechanisms [1]. Computations powered by algorithmic advances enable the generation and verification of realistic models that can be used to reveal new enzymatic catalysis mechanisms [2]. By using algorithmic tools for horizontal and vertical asymptotic analysis, enzymatic catalysis is regulated with a wide range of parameters in dimensional form with measurement precision [3]. Enzymes are transformed into biogenic robots with the signals sent to the biocatalyst, which maintains the enzymatic activity in the form of a continuous Markov chain ring by the parallel replication method by accelerating the stochastic reaction networks of the sinusoidal distribution. Rational catalyst design is determined by measuring the free energy changes in the Hamiltonian catalytic mechanism. Using programmable logic, Hamiltonian design defines free energy changes related to catalytic activity and input variables can be suggested by making uncertainty estimates. When the thermodynamic and kinetic parameters of the reaction mechanism calculated using empirical quantum chemistry are taken into account, enzymatic activity is achieved by jumps in small energy changes. As a result of the study, programmable bionic robot enzymes were created by combining quantum mechanics and Hamiltonian design and using free energy jumps.



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**KEYNOTE
SPEAKERS**

Day 2



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Apurba Bhattacharya

Texas A&M University, USA

Biography

Dr. Apurba Bhattacharya is a professor in the Department of Chemistry at TAMUK. Dr. Apurba Bhattacharya joined TAMUK in Fall, 1999. At the end of 2005, he took a leave of absence from TAMUK and served as the Global R&D Head and Senior Vice President in Dr Reddys Laboratories in India. He has over twenty years of experience in Pharmaceutical industry in the areas of drug delivery and drug development (prior to TAMUK) including Merck (8 yrs), Hoechst (8 yrs), Bristol Myers Squibb (2 yrs), and Dr. Reddy's Laboratories in India (2 yrs).

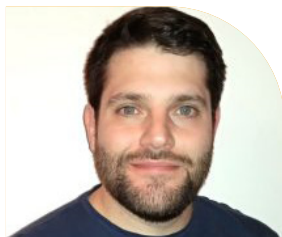
Research interests: Solvent Minimization, Reactions on Zeolite as Solid Support: Waste-free Catalytic Technology, Organic Reactions in Water, Atom-Economy, Energy conservation: Application of Microwave and Sonication in Organic Synthesis, Chiral Phase-Transfer Catalysis.

Green Chemistry in the Generic Pharmaceutical Industry

The Generic pharmaceutical industry accounts for nearly more than sixty percent of total prescriptions dispensed in the United States and approximately \$60 billion in revenues worldwide. The explosive growth in the Generic Pharmaceutical business also created environmental problems worldwide. Significant amounts of the chemistry that are practiced to produce the active pharmaceutical ingredients (API) are old, antiquated and waste producing. Over the past few years significant amount of research activities in the chemical community have been directed towards the development of new technologies and methodologies for environmentally benign processes. But unfortunately, the same has not been true for the Generic drug industry. Because the drugs are off patent, the innovator companies have no interest in modifying the chemistry and the Generic companies produce the drugs largely by following the existing patents with minimal change.

In Dr Reddys, we have been involved in developing processes for API's that have little or no pollution potential or environmental risk and are both economically and technologically feasible. We believe green synthesis will always be the most cost-effective synthesis at least in the long run. This Green Principle will be enunciated with examples of green syntheses that have been applied to several different API's including Rabeprazole, Finasteride, Levitiracetam, Galanthamine, Zafarlucastr and several others.

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Manuel Nuno

Vapourtec Ltd, UK

Biography

Dr. Manuel Nuño completed his MChem at Universidad de Zaragoza, Spain and York University, UK moving to University of Bath, UK to undertake his PhD in photocatalysis under the supervision of Dr Richard J. Ball.

Following completion of his PhD, Manuel advanced his process improvement skills during three years as process development chemist in food manufacturing industry working to improve the performance of large scale batch and flow chemical processes involving extraction, purification and crystallisation of sugars. Early in 2019 Manuel moved to Vapourtec Ltd as a research scientist, offering applications and chemistry support to customer and product development teams. Projects he has worked with include, photochemistry in flow, flow peptide synthesis, organometallic chemistry in flow and continuous electrochemical oxidation of natural products.

Catalytic processes under continuous flow – Current trends and applications

Flow chemistry is a growing area in modern chemistry. Thanks to its ability to perform faster reactions, ease of working with gases or unstable intermediates, flow chemistry has attracted a lot of interest for a wide variety of applications.

Probably one of the best-known advantages of flow chemistry is the ability to safely run high pressure-high temperature reactions (up to 200 bar), enabling to heat reactions over the solvents' boiling point. Flow reactions can then be completed within minutes, instead of hours when working in batch.

Catalysed reactions circumvent kinetics. By offering a lower energy pathway it does not require extreme conditions and works very well in round bottom flasks. Although it would not seem necessary to switch to a flow chemistry platform, the ability to work with gaseous reagents under pressure, the precise control of reaction conditions, or the wide range of inline analytical techniques, makes flow chemistry an ideal vehicle to explore catalysed processes.

The aim of this presentation is to describe different approaches to do catalysis in flow, covering the technical aspects, advantages, and how to choose the most suited approach. This presentation will cover examples from novel electrocatalysis to catalytic hydrogenations in both homogeneous and heterogeneous systems.

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Dana Stamo

University of Colorado Boulder, USA

Biography

Dana F. Stamo is a second-year Biological Engineering PhD student at the University of Colorado Boulder where she does research on novel therapeutics for hard-to-treat infectious diseases. In 2019, Dana graduated from the University of Colorado Boulder with her Bachelor's degree in Chemical & Biological Engineering. An artist in her free time, Dana often blurs the line between art and science, using creativity and design principles in her approach to engineering. When she isn't doing art or science, you'll find Dana hiking the Colorado Rockies, skating, or reading.

Light-Activated Quantum Dot Potentiation of Antibiotics to Treat Drug-Resistant Biofilms

Antimicrobial resistance is one of the biggest threats to global health and demands alternative therapies for multi-drug resistant (MDR) infections. Light-activated quantum dots (QDs) are a versatile candidate for treating MDR bacteria without harming mammalian cells. Furthermore, their ease of diffusion and ability to photo-potentiate allows for precise, localized treatment and their dynamic tunability keeps them in pace with bacterial evolution. While QDs are shown to be a viable alternative therapy for planktonic cultures, they have not been applied in treating bacterial biofilms (a common growth form that affords bacterial strains more resistance and persistence to immune and traditional drug attack). Additionally, the mechanism of QD attack—production of reactive oxygen species—and sub-breakpoint antibiotic treatments have been shown to stimulate biofilm formation, especially in clinical isolates. Herein, we demonstrate the previously observed mono-therapeutic stimulation of biofilm formation and apply QD-antibiotic combination therapies to overcome and nearly eradicate 48-hour, early-stage, static biofilms of *Escherichia coli* K12, methicillin-resistant *Staphylococcus aureus*, and *Pseudomonas aeruginosa*. These results lay the groundwork for QD-antibiotic combination treatments for late-stage clinical and industrial biofilms, contributing to the development of QD nanotherapeutics for combating MDR superbugs.

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Christo Boyadjiev

Bulgarian Academy of Sciences, Bulgaria

Biography

Professor Christo Boyadjiev was born on August 17, 1936. He graduated Higher Institute of Chemical Technology (Sofia) in 1960. His overall inventive career is inextricably linked with the Institute of Chemical Engineering and its predecessors – the Mass Transfer Processes Department in the Institute of General and Inorganic Chemistry at the Bulgarian Academy of Sciences (1963-1972) and the Central Laboratory of Theoretical Foundations of Chemical Engineering (1972-1986).

Currently, Professor is an Emeritus of Bulgarian Academy of Science – 2012 and Editor-in-Chief of the "Transactions of Academenergo" (Scientific journal of the Russian Academy of Science). And, also a member of Editorial Board for the "British Journal of Engineering & Technology"; Member of the Editorial Board for the "Transactions on Applied Chemistry"; Member of the Editorial Board for the SOP "Transactions on Physical Chemistry"; Review Board Member for the "Journal of Food Chemistry and Nutrition"; Chairman of the Scientific Council of the International Scientific Centre for Power and Chemical Engineering Problems.

A New Approach for Modeling of Catalytic Processes in Industrial Column Apparatuses

The industrial column catalytic reactors are possible to be modeled, using the new approach on the base of the physical approximations of the mechanics of continua. As a result, a convection-diffusion type model (for qualitative analysis) and an average-concentration type model (for quantitative analysis) are possible to be used for the catalytic processes modeling in column apparatuses, in the cases of physical and chemical adsorption mechanism. A numerical analysis shows, that average concentration model, where the radial velocity component is equal to zero (in the cases of a constant velocity radial non-uniformity along the column height), is possible to be used in the cases of an axial modification of the radial non-uniformity of the axial velocity component. The use of experimental data, for the average concentration at the column end, for a concrete process and column, permits to be obtained the model parameters, related with the radial non-uniformity of the velocity. These parameter values permits to be used the average concentration model for modeling of different processes in the cases of different values of the column height, average velocity, reagent diffusivity, chemical reaction rate constant, etc. This possibility will be used for modeling of the catalytic processes in a gas-solid column apparatus.

CATALYSIS AND CHEMICAL SCIENCE



Niels Ostyn

KU Leuven (KUL), Belgium

Biography

Niels Ostyn is doctoral researcher at KU Leuven in the Centre for Surface Chemistry and Catalysis, Characterization and Application Team (COK-KAT). He graduated at the University of Leuven in bioscience engineering with magna cum laude. His research expertise focuses on carbon materials, photocatalysis and materials characterization for the chemical functionalization and activation of graphene, graphite and carbon black. In the past, he performed an industrial internship at Total Research & Technology Feluy, where he worked on the improved preparation of graphene oxide for hydrotreating catalysts. He continued working on chemical modification of carbon materials in the research group of professor Johan Martens, studying the potential of heterogeneous photocatalysis. In the Martens group, he published three peer reviewed articles in high-impact international scientific journals. Niels is also an active member of The Young European Catalysis Network (YEuCat), in which he works together with young motivated researchers on challenging scientific themes.

Controlled graphite functionalization by photocatalytic oxidation for rationally engineered electrocatalysis

Graphene, graphite and graphite oxide are extraordinary carbon materials with superb physical and chemical properties such as thermal and electrical conductivity. These carbons are often described as the wonder materials of the 21st century. The number of high-end technological applications is expanding very rapidly. Liquid-phase chemical oxidation of graphite is the most prominent route towards oxidized graphite which has many interesting applications. These common wet chemical methods are however hazardous, produce lots of waste and do not allow handy control over the oxidation process and product. Efficient carbon based electrocatalyst design requires in particular a mild and controllable graphite oxidation process to provide a chemically tailored surface with moderate oxidation degree. Therefore, there is a need for a more sustainable oxidation enabling better control over the reaction, with spatial and temporal control, for fine tuning of the oxidized graphite. In this respect, we propose a vapor phase photocatalytic process for oxygen functionalization of graphite, presenting these technological advantages. Graphite is photocatalytically oxidized at low temperature using a TiO_2 photocatalyst, UV light and a gas mixture consisting of molecular oxygen and water vapor.

Our work aims at the best electrocatalysts design for energy-efficient electrochemical synthesis under mild conditions. A series of different carbon-based catalysts are investigated, since carbon materials often suppress undesired competing reactions while favoring charge transport. The electrocatalysts are prepared through a two-step synthesis process, in which the carbon support is first oxygen functionalized, using remote TiO_2 photocatalysis, and further activated by heteroatom doping. This highly controllable process enables to tune multiple catalyst design parameters (conductivity, metal loading etc.), enhancing the material's activity for electrochemical synthesis of valuable chemicals. To reveal all important material properties, the prepared catalyst is deeply looked into using advanced tools like electron microscopy and Raman and X-ray photoelectron spectroscopy.

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Alaa Hassan Al-Farttoosy

University of Basrah, Iraq

Biography

I have gotten B.Sc. In Agricultural Sciences- Plant Protection in 1999, my position was the fourth of Alumni of those years 1999 (the first quarter). Then I headed to complete the M.Sc. In the same department. Part of my project was done in the State Company of Petrochemical Industries in South of Basrah, while the second part was at the University of Basrah. In 2002, the first of October, I have got titled to an Assistant Agricultural Engineer. During this year, I was a postgraduate M.Sc. Student. In 2003, I have become an assist lecturer in the same department. Then I become gradually a Lecturer in 2006. After four years, I have got proportioned to an Assistant Professor of Pesticides. My early career as an academic at the University of Basrah in Iraq (2002-now) enabled me to develop a deep knowledge in pesticides and determination their residues using gas chromatography and the Mass- Spectrophotometry by undertaking both research and teaching activities. In 2015, I have gotten a scholarship to complete the PhD in the UK, Faculty of Engineering, Chemical and Biological Engineering Department. I was dedicated to my research work to study the microbial-based Bioremediation of Organophosphorus chemical warfare agent simulant Sarin. On 07-01-2020, I have finished my PhD viva to get the PhD certificate in the majority is In-situ bioremediation of Persistent Organic Pollutants (POPs) from water and soil.

Microbial-based Bioremediation of an Exemplar Organophosphorus Chemical Warfare Agent

Organophosphorus compounds are used as chemical warfare agents and pesticides, and can reside in the environment for a relatively long time, presenting health hazards. Hydrolysis rates of an exemplar OP compound, DEMP, were characterised in aqueous solutions in Chapter 3 and found to be stable under acidic conditions pH 6.0 at 25°C and neutral conditions pH 7.0 at 30°C. Rates could be increased by raising the temperature from 0.01 J Pain Relief ISSN: 2167-0846 JPAR an open access journa Fibromyalgia 2016 June 15-16, 2016 Volume 5, Issue 3(Suppl) Page 40 day⁻¹ at 25°C to 0.13 day⁻¹ at 35°C at pH 6.0, and at pH 7.0, the rates increased from 0.03 day⁻¹ at 25°C to 0.24 day⁻¹ at 35°C. Chapter 4 details how a bacterial consortium was successfully enriched from soil regularly exposed to organophosphorus pesticides. Initial DEMP degradation rates were improved from 0.010 h⁻¹ to 0.024 h⁻¹ following 12-months of adaptive evolution. From this consortium, three bacterial strains were isolated and identified via 16S rDNA barcoding as *Bacillus cereus*, *Micrococcus luteus*, and *Dermacoccus nishinomiyaensis*. Their growth and individual capability to degrade DEMP was evaluated, as well as in synthetic combinations, compared to control *E. coli* cultures and the enriched consortium. The growth rate of *M. luteus* was fastest at 1.52 day⁻¹ with a DEMP removal rate of 0.75 mg L⁻¹ day⁻¹. Fourier-transform infrared spectroscopy confirmed that the strains' isolates used DEMP during their growth. The strains *B. cereus* and *M. luteus* were also able to break down alternative organophosphorus compounds, namely triethyl phosphine-oxide, and tributyl phosphate. The enzymatic degradation by *B. cereus* was increased to 0.13 and 0.14 day⁻¹ for TEPO and TBP respectively. Furthermore, it has increased by using *M. luteus* in 0.12 of TEPO and 0.15 day⁻¹ of TBP. In contrast, the hydrolysis rates for TEPO 0.01 day⁻¹ and TBP 0.02 day⁻¹ after 21 days indicate that the hydrolysis of TEPO and TBP were low and slow. Our work aims at the best electrocatalysts design for energy-efficient electrochemical

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synthesis under mild conditions. A series of different carbon-based catalysts are investigated, since carbon materials often suppress undesired competing reactions while favoring charge transport. The electrocatalysts are prepared through a two-step synthesis process, in which the carbon support is first oxygen functionalized, using remote TiO_2 photocatalysis, and further activated by heteroatom doping. This highly controllable process enables to tune multiple catalyst design parameters (conductivity, metal loading etc.), enhancing the material's activity for electrochemical synthesis of valuable chemicals. To reveal all important material properties, the prepared catalyst is deeply looked into using advanced tools like electron microscopy and Raman and X-ray photoelectron spectroscopy.



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Christo Boyadjiev

Bulgarian Academy of Sciences, Bulgaria

Biography

Professor Christo Boyadjiev was born on August 17, 1936. He graduated Higher Institute of Chemical Technology (Sofia) in 1960. His overall inventive career is inextricably linked with the Institute of Chemical Engineering and its predecessors – the Mass Transfer Processes Department in the Institute of General and Inorganic Chemistry at the Bulgarian Academy of Sciences (1963-1972) and the Central Laboratory of Theoretical Foundations of Chemical Engineering (1972-1986).

Currently, Professor is an Emeritus of Bulgarian Academy of Science – 2012 and Editor-in-Chief of the "Transactions of Academenergo" (Scientific journal of the Russian Academy of Science). And, also a member of Editorial Board for the "British Journal of Engineering & Technology"; Member of the Editorial Board for the "Transactions on Applied Chemistry"; Member of the Editorial Board for the SOP "Transactions on Physical Chemistry"; Review Board Member for the "Journal of Food Chemistry and Nutrition"; Chairman of the Scientific Council of the International Scientific Centre for Power and Chemical Engineering Problems.

Reaction Kinetics in Chemical Engineering

In the lecture is presented a theoretical analysis of the role of the reaction kinetics in chemical engineering for the solution of the main problems in the chemical industry (biotechnology, heat energy), i.e. the optimal design of new devices and the optimal control of active processes. The thermodynamic and hydrodynamic approximations for the modeling of the industrial process rates are presented and analyzed.

The industrial processes are the result of reactions, i.e. creation or disappearance of a substance and (or) heat as a result of chemical and (or) physical processes and their rate is determined by the reaction kinetics.

The reactions deviate the systems from the thermodynamic equilibrium and as a result processes arise, who are trying to restore that equilibrium. The rate of these processes can be determined by Onsager's "linearity principle", where the rate of the process depends linearly on the deviation from the thermodynamic equilibrium.

The Onsager's linearity coefficient can be determined after solving the hydrodynamics, mass transfer and heat transfer equations, where it is proportional to the mass transfer (heat transfer) coefficient.

The relations between the Onsager's linearity coefficient and mass transfer coefficient are presented for different processes.



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