

# Catalysis Virtual 2020

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July 17-18, 2020

# CATALYSIS VIRTUAL 2020

JULY 17-18, 2020

**Theme:**

Exchange questions, answers, and best practices in the  
field of Catalysis

# INDEX

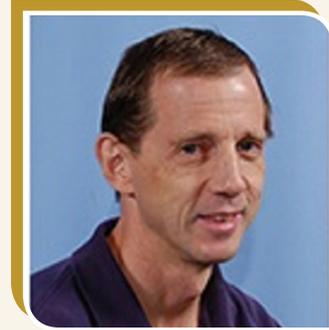
Contents	Pages
Keynote Speakers	4
About Host	5
Keynote Presentations	6
Oral Presentations	10
Poster Presentations	21
Participants List	25

# Keynote Speakers



Dave White

Climate Change Truth Inc, USA



Karl Sohlberg

Drexel University, USA



Dr. Sunirmal Jana

CSIR-Central Glass and Ceramic Research Institute, India

# *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* **Catalysis Virtual 2020** |

**Catalysis Virtual 2020** Webinar serves as a podium for the interaction between experts in the areas of Catalysis, Chemical Engineering & Technology around the world and aims in sharing some unique research and translational studies on various advances in the related fields. It is expected to bring together both reputable scientists in advanced stages of their career and young researches from many related disciplines. The webinar expects many new ideas to emerge at the interfaces between disciplines aiming to solve the most important problems relating to the Catalysis and Chemical Engineering. With its strong emphasis on innovative approaches, the webinar offers a chance for leading industry experts and scientists working in different areas of Catalysis and Chemical Engineering to learn new ideas that could help them advance their research and forge new professional relationships and collaborations. Our expert honorary speakers will provide you with the most clinically up-to-date relevant information you'll leave better educated and more invigorated than you thought possible.

# KEYNOTE FORUM

## CATALYSIS VIRTUAL 2020



WEBINAR

**Karl Sohlberg**

Drexel University, USA

## Modeling the thermal dependence of surface conductance in TiO<sub>2</sub> and MoO<sub>3</sub>: Refuting the bottleneck hypothesis

Surface conductance is a valuable tool to investigate the catalytic behavior of metal-oxide materials because adsorption/desorption of gases is frequently accompanied by charge transfer, which plays a central role in governing catalytic activity. A practical consequence of this relationship between adsorption and surface conductance is that surface conductance can serve as a useful proxy measurement for catalytic activity. Although the measurement of surface conductance is a macroscopic technique, its magnitude depends on the atomic-scale structures present on the surface of a material. Mathematical models that connect atomic-scale surface structure to surface conductance therefore provide a way to understand the surface structure of heterogeneous catalytic materials under realistic operating conditions. In particular, the thermal dependence of surface conductance contains information about the prevalence of binding sites and surface-adsorbed species. Non-Arrhenius thermal dependence of surface conductance has previously been reported for the transition-metal oxides TiO<sub>2</sub> and MoO<sub>3</sub>. The additional observation that conductance in these two materials depends on specific surface area has led to the hypothesis that the decreasing particle size that accompanies higher surface area leads to the formation of more inter-particle “bottlenecks” to charge transport, and consequently lower overall conductance. We will show, through the application of thermo chemical modeling, kinetic modeling, and analysis of equivalent resistance networks that this bottleneck hypothesis leads to predictions inconsistent with experimental observations.

Earlier work from our group showed that similar non-Arrhenius thermal dependence of surface conductance in the catalytic metal oxides  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> and SnO<sub>2</sub> may be described with a dual-charge-carrier model in which the contribution to charge transport by proton hopping across the surface is modulated by the prevalence of adsorbed water molecules. We will present a similar dual-charge-carrier model in which the adsorbate surface coverage is modulated by bi-Langmuir adsorption and apply it to TiO<sub>2</sub> and MoO<sub>3</sub>. This model captures well the thermal dependence of surface conductance in these materials, and predicts adsorption energies in very good agreement with published first-principles calculations. The results support the conclusion that the particle-size dependence of conductance in TiO<sub>2</sub> and MoO<sub>3</sub> likely arises from the increasing importance of surface processes to charge transport with decreasing particle size, not from an increase in the prevalence of inter-particle contacts.

### Biography

Dr. Sohlberg is an Associate Professor in the Department of Chemistry at Drexel University. His broad research area is theoretical and computational materials chemistry, with specific research programs in complex catalytic materials and molecular nano-devices. Before joining the Drexel faculty in 2000 he was an Oak Ridge Associated Universities postdoctoral fellow at Oak Ridge National Lab (Oak Ridge, TN). Earlier, he held postdoctoral appointments at The Johns Hopkins University and Brigham Young University. He received his PhD in physical chemistry from the University of Delaware under the supervision of Krzysztof Szalewicz. Sohlberg has more than 130 peer-reviewed publications.



## Dr. Sunirmal Jana

CSIR-Central Glass and Ceramic Research Institute, India

### Synthetic strategy and photocatalytic application of graphene hybridized metal oxide semiconductor nanocomposites

The biggest challenge of this 21st century is to solve the problem of environmental pollution especially water pollution. Now-a-days, water pollution related to contamination of organic dyes is a serious global concern and synthetic wastewaters from various dye industries including textile dyeing industry have posed a great threat to water environment. This problem could be mitigated by the use of metal oxide semiconductor (MOS) photocatalysts under light illumination. In this regard, many fundamental issues must have to be addressed to make the photocatalysts economically viable towards industrial application. It is worthy to note that the fast recombination of photogenerated electron-hole pairs as well as the mismatch of band gap energy and solar radiation spectrum limits the applicability of a MOS (like ZnO, TiO<sub>2</sub>). Several strategies have been adopted for making efficient MOS based photocatalysts including doping with anions/cations, improving surface structure by hybridizing / coupling with metals / other MOS / carbonaceous nanomaterials (like graphene, carbon nanotube, activated carbon, fullerenes) and increasing surface area, porosity as well as reactive facets of a photocatalyst.

In recent time, researchers are highly motivated to work upon a wide range of nanomaterials including graphene, boron nitride, black phosphorus, carbon nitride owing to their favourable physicochemical properties that are suitable for diverse applications in several potential fields including catalysis, energy storage, biomedical applications and so on. Among the nanomaterials, the research on graphene based nanomaterials is pioneer especially in the field of photocatalysis. It is known that graphene is a two-dimensional honeycomb structured and atomically thin carbonaceous material with exceptional functional properties. The research community commonly refers to its compounds include graphene oxide, reduced graphene oxide, highly reduced graphene oxide, chemically converted graphene as “graphene”. These compounds also able to form various functional nanocomposites (NCs) with inorganics (like metals, metal oxides) and organics (e.g. epoxy resin, polyaniline, polyvinyl alcohol). In our group, we have developed graphene hybridized inorganic/organic NCs such as ZnO-graphene hollow microspheres, europium incorporated ZnO-graphene nanocomposite, ZnO-graphene-polyaniline nanoflowers, Ag incorporated ZnO-graphene, polyethylene glycol capped Ag-ZnO-graphene, bovine serum albumin immobilized Au-ZnO-graphene NCs for different applications like cancer cell imaging, photocatalytic, photo-electrocatalytic, biomedical applications. The present talk will be focused upon the synthetic strategy and photocatalytic application addressing mechanistic pathways of wonderful graphene hybridized NCs with a special attention to graphene hybridized ZnO nanocomposites for remediation of organic dye contaminated water pollution.

#### Biography

Dr. Sunirmal Jana, Senior Principal Scientist & Professor at CSIR-Central Glass and Ceramic Research Institute (CSIR-CGCRI), Kolkata, India graduated as MS in Chemistry in 1991 from University of Kalyani and PhD (Science) in 1998 from Jadavpur University, India. He joined as a Junior Scientist at CSIR-CGCRI in December 1997. Dr. Jana worked as an invited Visiting Scientists including Brain Pool Scientist at Korea Research Institute of Chemical Technology, South Korea. He is an Editor/Editorial Board Member of several peer reviewed functional thin films and nanomaterials related journals. Dr. Jana is also a Life Member of many academic/research organizations/societies. Presently, he has published about 70 SCI/peer reviewed research papers, more than 80 conference papers, 6 book chapters and 3 Indian patents.



**Dave White**

Climate Change Truth Inc, USA

## Discovery: Reduction in photosynthesis correlation to Carbon dioxide increase

Carbon dioxide emissions correlate to 363ppm and are not the cause of the Atmospheric CO<sub>2</sub> rise since 1957. The correct cause is deforestation of the Amazon Rain-Forest (0.99 by Pearson's regression). Since 1950, the Amazon Rain forest has been deforested. An average of 12million hectare per year. This deforestation causes a minimum of 30% of the biomass burned. The burning of the biomass is adding billion of tons of carbon dioxide to the atmosphere. The carbon dioxide has overwhelmed the rain forest and caused massive decay. The rain forest has now become an oxygen sink and carbon dioxide producer. Now emitting 10billion tons of CO<sub>2</sub> annually. Also losing its ability to produce oxygen. To solve these issues the deforestation and burning needs to stop. Then after 10 years, the burning can continue 10% a year for 10 years. This will heal the Amazon and bring down atmospheric carbon dioxide quickly by increasing photosynthesis consumption to 100 billion tons annually. Stop non- sustainable deforestation like the Indian and Amazon rain forests. Please native trees and shrubs all over the world. The residence time of atmospheric CO<sub>2</sub> is 150 years. This is why there exists no signature to any recession or other lowering of CO<sub>2</sub> emissions.

### Biography

Dave is a Chemical Engineer with Masters Studies in Statistics, currently working on Climate Change. He has 30 years' experience since graduation in 1984. Promoting responsibility to environment and health of all species. Dave White graduated in Chemical Engineering in 1984. During the time at Oregon State University Dave worked on a cross flow counter current scrubber for coal fired power plants. Additionally took masters level classes on statistics. Then he moved to Hillsboro with his wife and worked in Semiconductors. In 2007 Dave along with Dr. Tom Wallow produced a paper on ArF double patterning for semiconductors. This multi-patterning scheme is widely used in today's semiconductor manufacturing plants. In 2011 Dave started a consulting business for Semiconductors. In 2017 Dave Started Climate Change Truth Research Inc. Dave is seeking the truth about climate change. His research interests are evaporation from the ocean, rain forest destruction effects and diffusion of CO<sub>2</sub> through the atmosphere.

# SPEAKERS

## CATALYSIS VIRTUAL 2020



WEBINAR



## Selective Nb<sub>2</sub>O<sub>5</sub> supported catalysts for the production of furfuryl alcohol and tetrahydrofurfuryl alcohol

Mayra Martinelli Costa  
University of Campinas, Brazil

Furfural (FUR) has been considered as one of the highest value-added compounds among biomass derivatives. Furfuryl alcohol (FA) and tetrahydrofurfuryl alcohol (THFA), furfural hydrogenation products, can be used in the production of resins, solvents, pharmaceutical products and other relevant chemicals. Metals Pd and Ni are often employed as catalytic active phase for liquid phase furfural hydrogenation. As for the support, Brazil is the world's leading niobium producer, with 88% of global production (US Geological Survey, 2019). Niobium pentoxide (Nb<sub>2</sub>O<sub>5</sub>) is a solid with interesting catalytic properties due the presence of Lewis and Brønsted acid sites. When used as a catalytic support, it may contribute to other reaction pathways, such as hydrodeoxydation (HDO). However, its use as catalytic support for furfural hydrogenation is still incipient. Therefore, the aim of this research is to evaluate the performance of Pd/Nb<sub>2</sub>O<sub>5</sub> and Ni/Nb<sub>2</sub>O<sub>5</sub> as catalysts for furfural hydrogenation in liquid phase. Niobium pentoxide was prepared by calcination of niobic acid (Nb<sub>2</sub>O<sub>5</sub>.nH<sub>2</sub>O) supplied by the Brazilian Metallurgy and Mining Company (CBMM). This procedure was carried out at 400°C for 4 h. The catalysts with 5 wt% metal were prepared by wet impregnation. Ni catalyst was reduced by H<sub>2</sub> flow (60 mL/min, 400°C, 3 h) and Pd catalyst was reduced by formaldehyde during the preparation procedure. Support and catalysts were characterized by N<sub>2</sub> physisorption (BET method), XRD and TPD-NH<sub>3</sub>. The reaction was carried out in a batch reactor, at 150°C and 5 MPa H<sub>2</sub>, using 2-propanol as solvent to reinforce the environmental purpose of this work. Reaction medium was analysed by gas chromatography. The support and catalysts exhibited predominantly amorphous structures according to XRD results, which enabled the synthesis of materials with specific surface area higher than 100 m<sup>2</sup>/g. Metallic Pd peaks were not observed in the diffractogram, which suggests that the reduction method on mild conditions led to the formation of small metallic crystallites. In turn, Ni catalyst presented 17 nm crystallites as estimated by Scherrer Equation. Also, all materials presented similar acid sites density (~5 μmol NH<sub>3</sub>/m<sup>2</sup>). Throughout the reaction catalysed by Pd/Nb<sub>2</sub>O<sub>5</sub>, complete furfural conversion was obtained and FA was hydrogenated to THFA. In contrast, catalyst Ni/Nb<sub>2</sub>O<sub>5</sub> presented 39% FUR conversion and a more constant selectivity towards FA, THFA was not observed. Additionally, the initial reaction rate was 12 times higher with the Pd catalyst, in comparison to the Ni catalyst. These results are in agreement with previous studies, which show Pd is highly active and usually more selective to THFA, while Ni is more selective to FA. Moreover, HDO product 2-methylfuran was observed only with Pd (selectivity <5%), which indicates that despite the acidity of the catalysts, the main reaction pathway was FUR hydrogenation.

### Biography

Ms. Costa possesses a bachelor's degree in Chemical Engineering from the University of Campinas, Brazil (2018). She is currently pursuing her Master's degree at the same institution under the supervision of Dr. Suppino. She developed a research project on catalysis at the Brazilian Synchrotron Light Laboratory (LNLS/CNPEM), which led to a publication in Chemical Engineering Transactions (Scopus Journal). Her most recent work regarding the use of niobia in heterogeneous catalysis was accepted for an oral presentation at the 17th International Congress of Catalysis.



## Electrospun materials for immobilization of oxidoreductases: Improving of their catalytic activity

Katarzyna Jankowska  
Poznan University of Technology, Poland

Nowadays, increasing amount of complex, hazardous compounds in surface waters is still unsolved problem. Therefore, defining new strategies of their conversion and removal from water is needed. In this case, enzyme immobilization could be solution of this problem because of properties of biocatalysts and possibility of their attachment onto support material and reuse them with relatively high activity. For environmental application, the most promising enzymes are oxidoreductases, especially laccases. These biomolecules, which are widespread in nature, catalyse the oxidation of a wide variety of organic compounds, such as dyes, pharmaceuticals and other phenolic compounds. Moreover, supports used in enzyme immobilization should be characterized by the presence of the key functional groups, 3-D structure, biocompatibility and stability in the reaction conditions. For this purpose, electrospinning technique seems to be one of the promising technologies for production of supports from various polymers and biopolymers with define structures and properties, enabling enzyme immobilization.

The main aim of the presented study was preparation of electrospun materials from polyamide 6 (PA6), polystyrene/poly (D,L-lactide-co-glycolide) (PS/PDLG) and polystyrene/cellulose acetate (PS/CA) and using them as potential supports for laccase immobilization. In order to study the properties of the obtained materials before and after laccase immobilization, scanning electron microscopy, Fourier transform infrared spectroscopy and UV-Vis spectrophotometry were used. The crucial step was evaluation of the catalytic activity of immobilized laccase on 3 selected support materials. In this case, model reactions with 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS) were conducted. The obtained electrospun fibers are characterized by 3-D structure and specific functional moieties, which enabled effective laccase immobilization. It should be noted that the highest catalytic activity of enzyme was observed after its attachment onto PS/CA fibers. It should be also stated that, for each of biosystem, relative catalytic activities were over 80% at specific reaction conditions: pH 5 and 25 °C. Moreover, laccase immobilized onto 3 materials could be used in 10 consecutive catalytic cycles with activity retention of over 70%. The presented results confirmed that the produced electrospun supports could be used in enzyme immobilization process.

**Acknowledgement:** This research was supported by research grant funds from the National Science Centre, Poland (2018/29/N/ST8/01026) and the National Agency of Academic Exchange, the Iwanowska Programme.

### Biography

MSc Eng. Katarzyna Jankowska studied Chemical Technology at Poznan University of Technology and graduated as MSc in 2017. She then joined the research group of Prof. Jesionowski at the Institute of Chemical Technology and Engineering at the same university. Biotechnology, enzyme immobilization and electrospinning technique are her scientific interests.



## Effect of metal loading on Nb<sub>2</sub>O<sub>5</sub> supported catalysts for the hydrogenation of furfural to furfuryl alcohol

Mayra Martinelli Costa  
University of Campinas, Brazil

Furfuryl alcohol, a furfural hydrogenation product, has important industrial applications, especially in the manufacturing of resins, for which it supplies thermal, mechanical and chemical stability. Recent studies indicate Ni as a promising active metal for the catalytic hydrogenation of furfural, as well as hydrodeoxygenation and decarbonylation. As for the choice of support, niobium pentoxide (Nb<sub>2</sub>O<sub>5</sub>) provides high specific surface area and porosity in addition to being vastly available in Brazil. Another important aspect of this solid is the natural presence of Brønsted and Lewis acid sites on its surface, capable of influencing its catalytic properties. Thus, in this work the performance of Ni/Nb<sub>2</sub>O<sub>5</sub> catalysts for the hydrogenation of furfural to furfuryl alcohol was evaluated. In order to obtain the support, niobic acid (Nb<sub>2</sub>O<sub>5</sub>.nH<sub>2</sub>O) supplied by the Brazilian Metallurgy and Mining Company (CBMM) was calcined at 400°C for 4 h. Catalysts with 10 wt% and 15 wt% Ni were synthesized by wet impregnation to investigate the influence of metal loading. The solids were activated under H<sub>2</sub> flow at 400°C for 3 h. The reaction was carried out in a batch reactor at 150°C and 5 MPa H<sub>2</sub> with 2-propanol as solvent, and the reaction medium was analysed by gas chromatography. The materials were characterized by N<sub>2</sub> physisorption (BET/BJH), EDS, DRX and TPD-NH<sub>3</sub>. It was observed a high agreement between the nominal metal loading of the solids and the result provided by EDS. The BET results show that Nb<sub>2</sub>O<sub>5</sub> has a specific surface area of 126 m<sup>2</sup>/g, adequate for its application as a catalytic support. Accordingly, the XRD results indicate a low degree of crystallinity of the solids. Peaks related to metallic Ni were identified by XRD, thus at least a portion of Ni was satisfactorily reduced. There was a gradual decrease in the specific surface area of the materials, as well as an increase in the mean pore diameter and average size of Ni crystallite, with the increase of metal loading. Such results suggest the occurrence of a partial blockage of the narrower pores as the amount of impregnated Ni increased, favoured by the presence of larger metallic crystallites. From the TPD-NH<sub>3</sub> results, it was observed that the acid sites density remained similar in all synthesized materials. Regarding the performance on reaction, the catalyst containing 15 wt% Ni showed a slight decrease in furfural conversion and initial reaction rate in comparison to the 10 wt% Ni catalyst. Such behaviour may be related to the textural properties of the material, which probably suffered loss of active sites on the surface. In addition, although the catalysts could be considered bifunctional as they retained the acidity of the support, the main reaction product was furfuryl alcohol, with selectivity between 50% and 70% throughout the reaction, in both cases. Despite Ni catalysts may favour other reaction routes as it is presented on the literature, this work presents a viable alternative to the production of furfuryl alcohol, using an accessible, easy to prepare catalyst.

### Biography

Ms. Costa possesses a bachelor's degree in Chemical Engineering from the University of Campinas, Brazil (2018). She is currently pursuing her Master's degree at the same institution under the supervision of Dr. Suppino. She developed a research project on catalysis at the Brazilian Synchrotron Light Laboratory (LNLS/CNPEM), which led to a publication in Chemical Engineering Transactions (Scopus Journal). Her most recent work regarding the use of niobia in heterogeneous catalysis was accepted for an oral presentation at the 17th International Congress of Catalysis.



## Catalytic conversion of lignin derived aromatic ethers under lignin-first conditions

Emilia Paone

Mediterranean University of Reggio Calabria, Italy

The reductive catalytic fractionation (RCF), widely known as “lignin-first” biorefinery, is emerging as an innovative approach to valorize the lignocellulosic biomass avoiding the alteration of the native structure of lignin thus allowing the production of added-value phenolic compounds [1-3]. The lignin-first approach involves solvolysis, fractionalization-depolymerization and reductive stabilization steps in the presence of a heterogeneous redox catalyst and a reducing agent using short chain alcohols or cyclic ethers in mixture with water as reaction medium. Traditional hydrogenation catalysts are generally adopted, being involved both in the depolymerization of the lignin structure as well as in the stabilization of monolignol and phenolic units.

The aim of this contribution is to investigate the basic chemistry beyond the lignin-first approach by using commercial available Ru/C and Pd/C catalysts for the C-O bond cleavage of lignin derived aromatic ethers. Diphenyl ether (DPE), Benzyl phenyl ether (BPE) and Phenethyl phenyl ether (PPE) were used to mimic, respectively, the 4-O-5, -O-4 and -O-4 lignin linkages [4, 5].

Catalytic tests were conducted in the presence of alcoholic H-donor solvents (methanol, ethanol and 2-propanol) or their mixture with water in the temperature range of 120-240°C both in the presence or in absence of molecular hydrogen as reducing agent. The Ru/C catalyst was found to be the best performing system with the less pronounced tendency to reduce the aromatic ring. The product distribution clearly shows that upon increasing the water content a decrease in the cleavage of C-O bond together with a higher aromatic production is observed. The best yield in aromatic compounds was obtained by using a 2-propanol/water mixture in absence of added molecular hydrogen, with the alcoholic solvent being the in situ H-source. Finally, deuterated 2-propanol-OD studies were conducted in order to elucidate the mechanism of transfer hydrogenolysis of DPE promoted by the Ru/C catalyst.

### Biography

Emilia Paone is a Post-Doc researcher at the Università degli Studi Mediterranea di Reggio Calabria, where she obtained her PhD in April 2019 working in the Chemistry Research Group. Her research activities lie in the field of heterogeneous catalysis with particular emphasis on the valorization of biomass derived molecules through the catalytic C-O bond breaking promoted by heterogeneous catalysts. In particular, her research project is focused in the catalytic transfer hydrogenolysis (CTH) of lignin for the sustainable production of aromatic feedstocks. Emilia Paone is co-author of 14 publications in peer-reviewed ISI journals and 2 ISI Book Chapters and, during these years, she attended as speaker several International and National Conferences.



## Combining biocatalysis and chemistry for the development of industrial processes

Lucia Steenkamp  
CSIR, South Africa

Consumers, through lifestyle changes demand new greener, environmentally friendly processes to produce final products on commercial scale including flavours and fragrances, pharmaceuticals and cosmetics. Extraction of some of these products from natural sources are time consuming and often yield product in small quantities. Biocatalysis and biotechnology can be used to replace the extractions as well as some harsh or dangerous chemical steps in the synthesis of intermediate and final products. Additional green chemistry steps are often required in a complete process. Three relevant technologies have been developed in the laboratories at the CSIR in South Africa. (-)-Ambrafuran, is used as a fixative agent that stabilises perfumes in formulations, by reducing the rate of evaporation of volatile substances and is therefore a scarce, valuable and sought-after perfumery material. The precursor, Ambergris is a metabolic product produced by the sperm whale (*Physeter macrocephalus* L.). Chemical synthetic routes have been developed in which (-)-ambrafuran is produced from sclareol in 8 steps employing some harsh and often very toxic chemicals with an overall yield of no more than 76%. A two step “green” route has been invented in our laboratory and sclareol extracted from the Clary sage plant, is converted to (-)-ambrafuran with an overall yield of up to 96%. The first step which eliminates 7 chemical steps involves a fermentation while the second step uses a benign zeolite.

The second example of a flavor and fragrance product combining biocatalysis and green chemistry is the production of l-menthol. The four diastereomers of menthol and their enantiomers, were synthesized by the hydrogenation of thymol to yield an eight isomer liquid menthol. A selective lipase reaction was developed to preferentially esterify l-menthol in hexane, hence simplifying separation from this diastereomeric mix through distillation. The final example involved the production of a pharmaceutical product and again biocatalysis and green chemistry were combined to synthesise (S)-naproxen, used as an inflammatory drug. Naproxen (2-(6-methoxy-2-naphthyl)-propionic acid) is widely used as a drug for human connective tissue diseases. As the (S)-enantiomer is 28-fold more active than the corresponding (R)-enantiomer, which also present unwanted side effects, it warranted the elimination of the (R)-enantiomer from the formulation. Classical chemistry was used to produce the racemate, followed by enantiomeric resolution of (R,S)-naproxen to yield the (S)-naproxen in high yield and enantiomeric excess using an esterase enzyme.

### Biography

Dr Lucia Steenkamp obtained her PhD in 1991 at the Rand Afrikaans University in Johannesburg, South Africa and was employed at Delta G Scientific and AECI before starting her career at the CSIR in 1999. She is a Principal Researcher and heads the Biocatalysis Group at the CSIR. She has 15 peer reviewed articles, 2 book chapters, 5 granted patents, 8 technology demonstrators and 5 complete Technology packages which were transferred and commercialized by industry partners. She won the award: South African Woman in Science for Research and Innovation in 2018.



## Comprehensive valorization of Agro-industrial waste via Green extraction: Futuristic food engineering

Owais Yousuf  
Integral University, India

In the present-day world of research and development, Agro Industrial waste valorization is still a broiling topic worldwide due to numerous facets of resource management, financial outlays and more prominently the food waste ecological impression. Agro waste, if handled suitably, can be treated for biogas and compost or can be used as feed stock but these are not the viable solutions for the sustainable future. As per reports, food processing industries account for roughly 39% of waste while food service sector augments 14% and 5% food waste occurs during food supply. Presently, a number of side-products of food processing industries like peel, pulp residue, stalk and seeds are considered invaluable by industry and are consequently left unexploited. Citrus peel is one of these processing industry waste which accounts for almost 40% of the total fruit weight for which several resources and energy is consumed to produce this share of plant material which consequently rests unutilized. Need and scope of waste valorization is well-known, but the finest means of achieving it are still being explored. One such promising and effective approach in resolving this problem is the Extraction of valuable products like bioactive compounds, pectin, essential oils, fibers, colorants etc. from agro industrial food waste but in contrary, existing extraction techniques possess several inadequacies in terms of economy, energy and longer time requirements. Consequently, these curbs, have led to the thoughtfulness of new “green” techniques in extraction, which usually use low costs and less energy. Furthermore, necessity is aimed at the design and development of the indigenous innovative extraction technique to overcome the problematical agro food waste of industries. As a result, technological enhancements need to be initiated in the agro industrial waste valorization to extract valuable constituents with least environmental impact and comprehensive reduction of “Agro Industrial Waste to No Waste”.

### Biography

Dr. Owais Yousuf is an Assistant Professor in the Department of Bioengineering, Integral University, Lucknow, India. His principal research and teaching interests encompasses the field of Food Engineering and Technology. He was awarded his Ph.D. (Process & Food Engineering) in 2019 from G. B Pant University of Agriculture & Technology, Pantnagar, India. Before perusing Ph.D., he has completed his M.Tech (Agricultural Process Food Engineering) from Aligarh Muslim University, Aligarh, India in 2014 and B.Tech (Food Technology) from Islamic University of Science & Technology, JK, India in 2012. He is an author of 12 research articles with several Citations. He is an ardent writer and a voracious reader and writes often for a number of magazines and newspapers as well. He is an Editorial Board member of numerous renowned journals and also serving as an eminent reviewer for several journals. He has actively participated in more than 30 Conferences, Workshops and Training programs at both National and International level. During his Doctoral program, he was selected by French ministry of agriculture under DEFIAA program for Two month training in Food Processing from various vocational and professional institutes of France.



## Clay modified with heteropoly acid (HPA) as environmental friendly catalyst for organic synthesis

Chandra Mohan

K. R. Mangalam University, India

Clays modified with Heteropoly acids (HPAs) have attracted much interest as heterogeneous catalysts for organic synthesis. For the present work, montmorillonite clay have been modified with three different heteropoly acids viz. Phosphotungstic acid (PTA), Silicomolybdic acid (SMA), Phosphomolybdic acid (PMA). HPA modified clays have shown improved qualities such as good thermal stability, high acidity and high oxidising ability as compared to the parent clay material. The high efficiency of these modified clay catalysts, can be compared with the other catalysts by using them in reactions such as Deoxygenation of oximes of aldehydes and ketones, synthesis of acetal derivatives of aldehydes and ketones, synthesis of coumarin derivatives etc.

These HPA modified clays have been found to be an efficient and reusable catalyst for the synthesis of variety of coumarin derivatives in excellent yields. These modified clays were characterized by various analytical techniques such as FT-IR, XRD, TGA, DSC etc. HPAs modified clays have been used as a highly efficient, reusable and environmental benign catalyst in some acid catalyzed reactions. Products were obtained in a moderate to high yields.

### Biography

Dr. Chandra Mohan obtained his Ph.D degree in the field of "Schiff based metal complexes and their applications as Chemical Sensors" from Guru Gobind Singh Indraprastha University, Delhi, India. He has done M.Phil in Inorganic Chemistry from Delhi University and performed his research work on "Heteropoly acid intercalated clays as catalysts" in 2009. He has keen interest in research and development activities. He has 8 years of teaching experience and about 8 years of research experience. He has published 15 research papers in reputed journals and has presented 10 research papers in various conferences and workshops held in India. He is an awardee of a national fellowship from University Grant Commission Delhi for his Ph.D. degree. He was also invited for a lecture from Sensor Lab, University of the Western Cape, Bellville, South Africa in May 2015 and as keynote speaker in the International conference at Imperial College London, UK in September 2018. Presently he is a reviewer & editorial member of 7 International Journals and 8 scientific bodies in India and abroad. He supervised one PhD student in 2018 and published more than 5 papers on recent COVID-19 pandemic in the year 2020. He has been involved in social welfare activities as NSS Coordinator and also worked on several projects based on COVID-19 outbreak.



## A Green approach for the synthesis of benzaldehyde using Zr/natural phosphate heterogeneous catalyst

Laasri Laila

Hassan II University of Casablanca, Morocco

**B**enzaldehyde is one of the most industrially useful aromatic aldehydes, it is used as a solvent in many industries and in the production of various pharmaceuticals, perfumes, flavorings, and dyes. According to the latest report on the global benzaldehyde market published in April 2020, the benzaldehyde sales will reach about 117 MT in 2023 with an annual growth of 3.18%. The air oxidation of toluene is the most used technique for the production of synthetic benzaldehyde, it requires extreme operating conditions and produces low yield. The oxidation of benzyl alcohol is another alternative to produce benzaldehyde that uses inorganic oxidants such as chromium salts or chlorinated substances often in organic media which suffer from poor selectivity and produce environmentally hazardous and toxic by-products. Currently, there is an urgent need for green alternatives processes for benzaldehyde production.

In this presentation, we report an environmentally friendly synthesis of benzaldehyde by oxidizing benzyl alcohol in solventless condition, by using H<sub>2</sub>O<sub>2</sub> as green oxidant, and Zr/Natural Phosphate as catalyst producing water as by-product. Optimization Conditions were conducted using full factorial experimental design. A maximum yield of 85% was obtained under the optimal reaction conditions. The catalyst can be recovered by simple filtration and reused over four consecutive cycles without a significant loss in its activity.

To evaluate the potential environmental acceptability of the developed process, we determined a set of green metrics (atom economy (AE), E-Factor, reaction mass efficiency (RME), stoichiometric factor (SF), material recovery parameter (MRP)), and we assessed the conformity to green chemistry principles.

### Biography

Dr. Laila LAASRI is currently Professor at the Faculty of Sciences Ben M'Sik, Casablanca, Morocco since 2013. She was awarded her PhD in 2007 from the University of Hassan II of Casablanca, Morocco. She then worked in an engineering school, ESITH-Casablanca, where she held the position of R&D Director. Her research interests include the introduction of green organic chemistry in laboratory describing the environmentally benign preparation of highly added value products, while enhancing natural phosphate as an efficient heterogenous catalyst and a very abundant Moroccan natural resource. The author holds two patents related to the valuation of Moroccan natural resource.



## Preparation of activated carbons from biomass and application as a support for silver nanoparticles in bacterial depollution

Dounia Elbasyouni  
University Blida, Algeria

In recent years, there has been a particular interest in preparation of activated carbon as a catalyst, using agricultural products as raw material, which are considered as renewable natural resource with a low price in order to valorize local material and preserving the environment from solid waste. The activated carbons showed a high efficacy in water treatment, and gas purification. The activated carbon, which we produced using date's cores by long process, simulated the high physiochemical and antimicrobial properties of silver nanoparticles especially in antibacterial activities for water purification against *Escherichia coli* and *Pseudomonas aeruginosa*, which is one of the most environment issues and public health. Silver nanoparticles recognized since long term for its inhibitory effect on bacteria in medical environment and industrial process environment. We produced silver nanoparticles by two economic methods, which are the chemical method (polyol), and the green method using black tea leaf extract. Moreover we have applied a technic where the silver nanoparticles are directly supported with two types of activated carbon one which we prepared by date's cores (figure1), and the second is commercial from the market. In addition, we compared the results between the prepared and the commercial activated carbon; furthermore, we compared the efficacy between the chemical and the green method for producing silver nanoparticles. This study will also permit us to find new water sources by reuse wastewater after is purified at very low coast, and even will help purifying seawater, dam water and rivers water, convert sewage into suitable water for irrigation also purifying hospital's wastes, promote preventing ecological and biological disasters in low price.

### Biography

My name is Dounia Elbasyouni, I am a recent college graduate, I finished my master degree in Process Engineering of Materials. At my last year in college I worked on "Preparation of activated carbons from biomass and application as a support for silver nanoparticles in bacterial deppollution" project. And now am searching for a PhD scholarship. I always keep my goals and tasks arginized to maintain productivity. I believe that the skills that I have attained from the dynamic environment and competitive university life define me and I am looking forward to implementing and polishing them in any opportunity that I receive.



## Environmentally friendly synthesis of catalyst based on chitosan for the degradation of phenolic contaminants

Julieta Lorena Sacchetto

Universidad Nacional de Río Cuarto, Argentina

The main degradation pathways for pollutants are chemical ones, which include those transformations that take place in the presence of solar radiation, known as direct or indirect photoreactions. In this work, the focus will be on sensitized photolysis reaction, it requires the presence of another molecule, a dye, which will absorb light radiation and produce excited states with the ability to initiate a cascade of photoprocesses in which highly reactive species are generated. The main problem with these processes lies in removing the dye once the reaction is complete. With the use of polymeric dyes (PD) whose water solubility varies with the solution's pH this issue can be minimized or completely resolved since it allows its extraction, after being used in the removal of contaminant, with a simple change of pH in the medium.

The polymeric dye is composed by two natural reactive, principally the sensitizer flavin mononucleotide (FMN) and the chitosan (CH). Among other relevant characteristics, we can mention: they are biomolecules, non-toxic, biocompatible, food and cosmetic additives, which makes CP completely friendly to aquatic environments. For CP synthesis, 1-Ethyl-3-(3-dimethylaminopropyl) carbodiimide (EDC) was used to crosslinker, to produce a phosphoramidate bond through EDC, which is formed from the phosphate group of FMN and the amino group of CH. A polymer of the same colour and similar photo physical properties of FMN was obtained.

Another relevant characteristic of this PD is that it is more photostable than the free dye and is easily extracted from the medium by pH change, since it is soluble in acetic acid solution and precipitates in pH solution  $> 5.9$ . To evaluate the photocatalytic activity of the synthesized polymer, trihydroxybenzenes (THB) compounds were chosen. THB are recognized pollutants and in homogeneous media are reactive towards singlet oxygen ( $^1O_2$ ). The photosensitized degradation of THBs by CP was monitored by oxygen consumption and UV-Vis spectroscopy. In all cases, the presence of THB increases the rate of oxygen consumption when irradiating the CP solution alone. On the other hand, spectral changes were recorded in the irradiated solutions. To determine the reactive oxygen species in the degradation mechanism different specific inhibitors were used. These experiments show the participation of  $^1O_2$ ,  $H_2O_2$  and hydroxyperoxyl radicals in the THBs degradation. Furthermore, laser flash photolysis experiments showed that the electronically excited states of CP also participate in THB degradation. The use of a photosensitized heterogeneous system represents a great advantage over homogeneous systems. On the other hand, the CP has a greater photostability, which allows it to be used for longer times, and on the other hand, it is the most promising of these CP, is that it can be extracted after photosensitized reaction, leaving the aquatic environments without contaminants or dyes.

### Biography

Julieta Lorena Sacchetto studied Chemistry at the Universidad Nacional de Río Cuarto, Argentina and graduated as MS in 2017. She joined the Photochemistry and Environment research group of Dr. Walter A Massad at the Instituto de Desarrollo Agroindustrial y de la Salud (IDAS) CONICET-UNRC. In 2017, she worked as a quality assistant at SGS Argentina S.A. She is doing her PhD degree, she started in 2018 at the same institution. She has published 6 articles in national and international conferences.

# POSTERS

## CATALYSIS VIRTUAL 2020



WEBINAR



## Kinetic study of catalytic hydrogen evolution and 4-nitrophenol reduction reactions on Ag-Pt bimetallic nanoparticles

Shalaka Varshney  
Ariel University, Israel

**M**etallic nanoparticles (NPs) have gained a massive interest as catalysts and been a subject of extensive research.<sup>1-2</sup> Herein, we present a comprehensive kinetic study of two competitive reactions: hydrogen evolution reaction (HER), and the reduction of 4-nitrophenol to 4-aminophenol. The investigated catalysts were Ag, Au, Pt metallic and Au-Pt, Ag-Pt bimetallic alloy NPs that were synthesized in aqueous suspensions without using any added stabilizer and the reducing agent was NaBH<sub>4</sub>. Owing to synergism between the metals in the alloy NPs, those have shown superior catalytic performance compared to other reported metallic and bimetallic NPs. Ag-Pt (9:1) NPs display them both as a low-cost and highly efficient reduction catalyst with an apparent rate constant of  $59 \times 10^{-3} \text{ s}^{-1}$  and an extremely high activity parameter value of 13,600 s<sup>-1</sup>g<sup>-1</sup> with only 10% of the expensive Pt. This high activity parameter value is being reported for the first time. Kinetic study of hydrogen evolution on various metallic and bimetallic NPs was conducted in parallel to the reduction of 4-nitrophenol, and from this competition, new mechanistic insights were derived. High-resolution transmission electron microscopy (HR-TEM), X-ray powder diffraction (XRD), and X-ray photoelectron spectroscopy (XPS) studies show that the silver-rich Ag-Pt alloy NPs have a spherical linked shape with the size of ~4.0 nm and confirms the structure of an alloy.

### Biography

Shalaka Varshney was born in Uttar Pradesh, India in 1993. She is a PhD student at the Department of Chemical Sciences, Ariel University, Ariel, Israel under the supervision of Dr. Tomer Zidki and Prof. Dan Meyerstein. She received her Dual Degree B.Tech. and M.Tech. in Nanotechnology from the University of Rajasthan, Jaipur, India in 2016. Her research currently focuses on the investigation of nanocatalytic reaction mechanism on the surface of metallic and bimetallic nanoparticles catalyzed reduction reactions. Her interests are in the synthesis and characterization of metallic, bimetallic nanoparticles and different dimensional nanomaterials and their self-assembly in discotic liquid crystals.



## Removal of chlorophenols from aqueous solutions using membrane/electrospun fibers/laccase system

Katarzyna Jankowska

Poznan University of Technology, Poland

**P**ulp paper industry is one of the most polluting industry in the world, which is releasing wastewaters containing very complex organic and inorganic pollutants. Among hazardous compounds such as phenols, organic halogens and polychlorinated biphenyls, one of the most dangerous chemicals for environment and human health are chlorophenols. They can cause severe toxicity to aquatic life and serious threat for human, such as cancers, allergies and neurological disorders. There are a number of methods used to remove chlorophenols from aqueous solutions, such as photocatalysis or membrane techniques, however more effective ways of their degradation are still being sought. In this case bimodal removal of these compounds, using simultaneous biocatalysis and membrane separation, seems to be a promising method of effective conversion and removal of chlorophenols from aqueous solutions.

In the presented work 2-chlorophenol and 4-chlorophenol were degraded using membrane/electrospun fiber/laccase system. In this case, the ultra filtration membrane was covered by electrospun cellulose acetate (CA), using direct-spraying method. After that, membrane with electrospun fibers was used as a support for laccase immobilization by adsorption method. Based on the obtained results, it was confirmed that the support was obtained efficiently, and the laccase was immobilized successfully. The crucial step of the presented investigation was removal study of 2-chlorophenol and 4-chlorophenol at various process conditions. Effects of the concentration of chlorophenol solution, pH and temperature conditions on the efficiency of enzymatic conversion and membrane separation were evaluated using UV-Vis spectroscopy with derivatization using reaction with 4-aminoantipyrine (4-AAP). What is more, it was found that it is possible to reuse the biocatalytic systems produced in successive degradation cycles.

**Acknowledgement:** This research was supported by research grant funds from the National Agency of Academic Exchange, the Iwanowska Programme.

### Biography

MSc Eng. Katarzyna Jankowska studied Chemical Technology at Poznan University of Technology and graduated as MSc in 2017. She then joined the research group of Prof. Jesionowski at the Institute of Chemical Technology and Engineering at the same university. Biotechnology, enzyme immobilization and electrospinning technique are her scientific interests.



## Optimising the in vivo biocatalysis of oxygenated and acetylated Taxol precursors in *Saccharomyces cerevisiae* using advanced bioprocessing strategies

Leonardo Rios Solis

University of Edinburgh, United Kingdom

**T**axadien-5 $\alpha$ -hydroxylase and taxadien-5 $\alpha$ -ol O-acetyltransferase catalyse the oxidation of taxadiene to taxadien-5 $\alpha$ -ol and subsequent acetylation to taxadien-5 $\alpha$ -yl-acetate in the biosynthesis of the blockbuster anti-cancer drug, paclitaxel (Taxol). Despite decades of research, the promiscuous and multispecific CYP725A4 enzyme remains a major bottleneck in microbial biosynthetic pathway development. In this study, an interdisciplinary approach was applied for the construction and optimisation of the early biocatalytic pathway in *Saccharomyces cerevisiae*, across a range of bioreactor scales. High-throughput microscale optimisation enhanced total oxygenated taxane titre to  $39.0 \pm 5.7$  mg/L and total taxane product titres were comparable at micro and mini-bioreactor scale at  $95.4 \pm 18.0$  and  $98.9$  mg/L, respectively. The introduction of pH control successfully mitigated a reduction of oxygenated taxane production, enhancing the potential taxadien-5 $\alpha$ -ol isomer titre to  $19.2$  mg/L, comparable to the  $23.8 \pm 3.7$  mg/L achieved at microscale. A combination of bioprocess optimisation and increased GC-MS resolution at 1L bioreactor scale facilitated taxadien-5 $\alpha$ -yl-acetate detection with a final titre of  $3.7$  mg/L. Total oxygenated taxane titres were improved 2.7-fold at this scale to  $78$  mg/L, the highest reported titre in yeast. Critical parameters affecting the productivity of the engineered strain were identified across a range of scales, providing a foundation for the development of robust integrated bioprocess control systems.

### Biography

Dr Rios is a Lecturer at the Institute for Bioengineering at the School of Edinburgh with more than 10 years of proven track record in Biocatalysis, Synthetic Biology and Biochemical Engineering. His research group has ample expertise in precision genome engineering and enzyme engineering combined with using high-throughput automated microscale tools. Dr Rios is currently the director of the Bio-automation network at the University of Edinburgh. Dr Rios is also currently representing the UK in the Management Committee of the European Union Coordination Support Action (CSA) project "BioRoboost" setting up an international collaborative network on synthetic biology and automation standards.

## PARTICIPANTS LIST

Name	P No.
<b>Chandra Mohan</b> K R Mangalam University, India	17
<b>Dave White</b> Climate Change Truth Inc, USA	9
<b>Dounia Elbasyouni</b> University Blida, Algeria	19
<b>Emilia Paone</b> Mediterranean University of Reggio Calabria, Italy	14
<b>Julieta Lorena Sacchetto</b> Universidad Nacional de Río Cuarto (UNRC), Argentina	20
<b>Karl Sohlberg</b> Drexel University, USA	7
<b>Katarzyna Jankowska</b> Poznan University of Technology, Poland	12, 23
<b>Laasri Laila</b> Hassan II University of Casablanca, Morocco	18
<b>Leonardo Rios Solis</b> University of Edinburgh, United Kingdom	24
<b>Lucia Steenkamp</b> CSIR, South Africa	15
<b>Mayra Martinelli Costa</b> University of Campinas, Brazil	11, 13
<b>Owais Yousuf</b> Integral University, India	16
<b>Shalaka Varshney</b> Ariel University, Israel	22
<b>Sunirmal Jana</b> CSIR-Central Glass and Ceramic Research Institute, India	8



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