Coalesce Research Group

Webinar on

BIOCATALYSIS & GREEN CHEMISTRY

June 24-25, 2021 | 12:00 - 18:00 (British Time)

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Scientific Program

Webinar on

Biocatalysis & Green Chemistry

Thursday
June 24, 2021

	Day 1 - June 24, 2021 - British Time
12:00 - 12:15	Introduction
	Oral Presentations
12:15 - 12:40	Surface adsorption - biocatalysis *via* immobilized phospholipase D to produce phosphatidylserine without toxic organic reagents **Binglin Li,** Northwest University, China
12:40 - 13:05	Chemo-enzymatic synthesis of L - menthol **Gang Xu,** Zhejiang University, China
13:05 - 13:30	Electrocatalytic transformation of biomass for chemicals and fuel production as climate change mitigation strategies **Chun Ho Lam,** City University of Hong Kong, Hong Kong
	Lunch (13:30 - 14:00)
14:00 - 14:25	Teaching iron to perform like palladium in cross coupling reactions **Jordi Poater,** Universitat de Barcelona, Spain
14:25 - 14:50	Influence of heterocyclic ligands on catalytic properties of oxovanadium(IV) complex compounds in olefin oligomerization **Joanna Drzeżdżon,** University of Gdansk, Poland
14:50 - 15:15	Supercritical water gasification with lignocellulosic biomass waste as the feedstocks - Economic analysis of noncatalytic SCWG at 600°C versus catalytic SCWG at 400°C **Chai Siah Lee,** University of Nottingham, United Kingdom
15:15 - 15:40	Rosemary essential oils as a promising source of bioactive compounds: Chemicalprofile, biological activity, thermal properties, and possibility of utilization as antioxidant agent **Saša Đurović,** Institute of General and Physical Chemistry, Serbia
15:40 - 16:05	Artificial metalloenzymes based on vancomycin for stereoselective catalysis in aqueous media **Facchetti Giorgio,** University of Milan, Italy
16:05 - 16:30	A highly efficient two - step “Green” process for (-) ambrafuran production **Lucia Steenkamp,** CSIR, South Africa
16:30 - 16:55	Purple non - sulfur photosynthetic bacteria as a source of biohydrogen and bioplastics **Eleftherios Touloupakis,** National Research Council, Italy
16:55 - 17:20	Preparative redox transformations of carbonyl compounds catalyzed by the whiterot fungi **Tatyana Zhuk,** Justus Liebig University Giessen, Germany
17:20 - 17:45	Liver - targeting class I selective histone deacetylase inhibitors potently suppress hepatocellular tumor growth as standalone agents **Bocheng Wu,** Georgia Institute of Technology, USA
17:45 - 18:10	Swelling kinetics and thermal properties of hydrogels composed of n - butyl acrylate and isobornyl acrylate **Ahlam Benkhelifa,** University of Tlemcen, Algeria
	End of Day 1 Sessions

Scientific Program

Webinar on

Biocatalysis & Green Chemistry

Friday

June 25, 2021

Day 2 - June 25, 2021 - British Time

	Keynote Presentation
12:00 - 12:30	Curcumin as a novel reducing and stabilizing agent for the green synthesis of metallic nanoparticles for their catalytic applications **Digambara Patra,** American University of Beirut, Lebanon
	Oral Presentations
12:30 - 12:55	Photoelectrochemical reduction of N_2 to NH_3 under ambient conditions through hierarchical $MoSe_2$@g - C_3N_4 heterojunctions **Muhammad Asim Mushtaq,** Beijing University of Chemical Technology, China
12:55 - 13:20	Composite nanofibers for improved photocatalytic performance under UV and visible light irradiation **Mirela Suchea,** Hellenic Mediterranean University, Greece
	Lunch (13:20 - 13:45)
13:45 - 14:10	Typha angustifolia, a beneficial plant for waste water treatment **I.C. Covaliu,** Polytechnic University of Bucharest, Romania
14:10 - 14:35	Biocatalytic approach for direct esterification of Ibuprofen with sorbitol in biphasic media **Federico Zappaterra,** University of Ferrara, Italy
14:35 - 15:00	Composite core @ shell microgel particles for catalytic reduction of toxic nitroarenes **Khalida Naseem,** University of Central Punjab, Pakistan
15:00 - 15:25	Towards an ideotype for food-fuel dual-purpose wheat in Argentina **Maria Mercedes Echarte,** National Institute of Agricultural Technology, Argentina
15:25 - 15:50	Biologically plant - based pigments in sustainableinnovations for functional textiles – The role of greenchemistry **Alka Madhukar Thakker,** Heriot - Watt University, UK
15:50 - 16:15	Removal persistent pollutants by Fenton systems: Enhancing degradation by bio - based chelating agents **Romina Romero,** Universidad de Tarapacá, Chile
	Keynote Presentation
16:15 - 16:40	Tailoring diffusive pathways and thermal expansion in Ti - alloys **Matthias Bönisch,** KU Leuven Leuven, Belgium
	Poster Presentations
16:40 - 16:50	Catalytic activity of plasma - prepared thin films based on mixed cobalt and iron oxides in CO2 conversion to CO **Ryszard Kapica,** Lodz University of Technology, Poland
16:50 - 17:00	Catalytical activity of tungsten - containing thin films deposited by plasma enhanced chemical vapor deposition method **Aleksandra Kędzierska - Sar,** Lodz University of Technology, Poland
17:00 - 17:10	Biologically plant - based pigments in sustainable innovations for functional textiles – The role of bioactive plant phytochemicals **Alka Madhukar Thakker,** Heriot - Watt University, United kingdom

Webinar on

Biocatalysis & Green Chemistry

Friday
June 25, 2021

Oral Presentation	
17:10 - 17:30	Novel Glycosylated Histone Deacetylase Inhibitors For Targeted Treatment Of Hepatocellular Carcinoma **Bocheng Wu,** Georgia Institute of Technology, USA
Video Presentations	
17:30 - 17:45	Surfactant - free colloids: Greener syntheses for nanoparticle and nanocatalysts **Jonathan Quinson,** University of Copenhagen, Denmark
17:45 - 18:00	Greenhouse covering plastics films waste management: A case - study GIS - based model **Monica Parlato,** University of Catania – Di3A, Italy
End of Day 2 Sessions	

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Day 1
Oral Sessions

SURFACE ADSORPTION-BIOCATALYSIS *VIA* IMMOBILIZED PHOSPHOLIPASE D TO PRODUCE PHOSPHATIDYLSERINE WITHOUT TOXIC ORGANIC REAGENTS.

Binglin Li, Jiao Wang and Xiaoli Zhang

Northwest University, China

Abstract

Background: The adsorption of substrates/products on immobilized enzymes was a common bad phenomenon. A novel method was proposed to turn this “drawback” into treasure. Immobilized phospholipase D (PLD) acted as not only the catalyst, but also an “anchor molecule” facilitating the adsorption of hydrophobic substrate phosphatidylcholine (PC) in purely aqueous solutions and smoothly entering into transphosphatidylation.

Objective: Efficient production of phosphatidylserine in a green way.

Methods: PLD proteins were covalently immobilized on silica. The content of PLD on the carrier surface was controlled at 1.75 $mg_{protein}/g_{silica}$. Immobilized PLD was resuspended in acetate buffer (pH 6.0) with 0.2 $_{gcatalysis}$/mL. One milligram of PC was dispersed in 2 mL of 0.2 M acetate buffer (pH 6.0) in an ultrasonic bath for 15 min, and the obtained solution was stirred (500 rpm) for 6 h. Then, 200 mg of L-serine were dissolved in the above mixture. Immobilized PLD solution (0.1 mL) was added to activate the reaction at 35 °C.

Results: The PC loading even reached 96.7%. The adsorption region and relevant driving forces were confirmed by the molecular docking and dynamics. The highest yield of phosphatidylserine (PS) reached 95.4%. An “artificial interphase” was created, allowing a hydrophobic microenvironment for minimal hydrolysis. Biomolecular simulations indicated that adsorbed PC molecules would diffuse into the active center by rapid adsorption-desorption equilibrium or the parallel movement on the surface of PLD or combination diffusion. It explained why these “fixed” substrates could interact with the active center. Moreover, obtained PS was manufactured into microcapsules and toxic solvents were completely avoided in the whole process.

Biography

Binglin Li has his expertise in the biocatalysis for the production of naturally rare or non-natural phospholipids. He is devoting to develop the green and efficient system for phospholipase D-catalyzed transphosphatidylation. Several aqueous-solid systems were constructed to reduce or avoid the use of the toxic organic solvents. The safety of product was significantly improved. In this work, an environmentally friendly and highly efficient system was constructed for the production of PS by the surface adsorption-catalysis. Relevant mechanisms were systematically investigated by the biomolecular simulation.

CHEMO-ENZYMATIC SYNTHESIS OF *L*-MENTHOL

Gang Xu

Zhejiang University, China

Abstract

L-menthol is the world's largest flavor additive, and its demand is still increasing rapidly. There have been many synthetic routes for menthol, such as hydrogenation of thymol to synthesize menthol. However, it is still a challenge to obtain optically pure *L*-menthol from the eight isomers. Herein, the chemical-enzymatic cascade and site-specifically incorporate unnatural amino acids were used to obtain optically pure *L*-menthol. In the chemical synthesis step, we prepared solid superbase K_2O-Al_2O_3 by loading alkali metal salt on γ-Al_2O_3. Employing its selective transesterification ability to increase the content of *L*-menthol propionate for the subsequent enzymatic resolution process. Then, in the enzymatic resolution step, lipase (*Pa*L) produced by *Pseudomonas alcaligenes* was used to resolve eight menthol propionate isomers to obtain *L*-menthol. It was modified by incorporating unnatural amino acids and substitution of Ala253 with o-bromophenylalanine had the highest diastereomer selectivity (>95%) at a high *L*-menthol propionate conversion rate (>94%).

Biography

Gang xu is associate professor of the College of Chemical and Biological Engineering Zhejiang University and got Ph. D. of Organic Chemistry in Zhejiang University in 2005. In 2016, he studied 1year in the School of Pharmacy of Mississippi University as visiting scholar. His research interests are mainly about the efficient construction of chiral chemical compound by Chemo-Enzymatic method.

ELECTROCATALYTIC TRANSFORMATION OF BIOMASS FOR CHEMICALS AND FUEL PRODUCTION AS CLIMATE CHANGE MITIGATION STRATEGIES

Chun Ho Lam and Qingshi Tu
City University of Hong Kong, Hong Kong

Abstract

Background: The manufacture of goods from oil, coal, or gas to everyday consumer products comprises in more or less all cases at least one catalytic step. Compared to conventional hydrothermal catalysis, electrocatalysis possesses the advantage of mild operational conditions and high selectivity, yet the potential energy savings and climate change mitigation have rarely been assessed. This study conducted a life cycle assessment (LCA) for the electrocatalytic oxidation of crude glycerol to produce lactic acid, one of the most common platform chemicals. The LCA results demonstrated a 31% reduction in global warming potential (GWP) compared to the benchmark (bio- and chemocatalytic) processes. Additionally, electrocatalysis yielded a synergetic potential to mitigate climate change depending on the scenario. For example, electrocatalysis combined with a low-carbon-intensity grid can reduce GWP by 57% if the process yields lactic acid and lignocellulosic biofuel as compared to a conventional fossil-based system with functionally equivalent products. This illustrates the potential of electrocatalysis as an important contributor to climate change mitigation across multiple industries. A technoeconomic analysis (TEA) for electrocatalytic lactic acid production indicated considerable challenges in economic feasibility due to the significant upfront capital cost. This challenge could be largely addressed by enabling dual redox processing to produce separate streams of renewable chemicals and biofuels simultaneously.

Objective: To discuss how electrocatalytic provides a novel pathway to produce chemicals and to quantitatively demonstrate its potential to reduce greenhouse gas emission.

Methods: The electrocatalytic synthesis of lactic acid from glycerol and the separation unit operations were modeled in AspenPlus® v8.1. Process parameters such as feed, reaction temperature and pressure were obtained from the optimum laboratory conditions Experimental data of material, energy and waste flows was fed to both a TEA model and a LCA model for evaluating the metrics of interest (e.g., net present value, global warming potential).

Results: (Key finding) The GWP result of the electrocatalytic oxidation pathway under a nominal configuration (i.e., assuming no uncertainty associated with the operation conditions) was 38.6 kg CO_2-eq, which is approximately 31% and 40% lower than the benchmark (hybrid bio-/chemo-catalytic pathway: 56.0 kg CO2-eq) and conventional (fermentation of glucose: 64.5 kg CO_2-eq) results, respectively.

Conclusion: The results demonstrated the advantage of electrocatalytic system over the baseline system in terms of total reduction in climate change impacts, but also showed how the two different systems (hybrid bio-/chemo-catalytic pathway and fermentative pathway). In general, the milder operation conditions of electrocatalysis-based technologies could lead to overall savings in energy and hence, reducing climate change impacts from a life cycle perspective. In addition, electrocatalysis-based technologies could increase the share of electricity in the energy consumption patterns for different manufacturing processes, which augmented the benefits of promoting low carbon intensity electricity.

Biography

Dr. Chun Ho (Jason) Lam's research explores how biomass and organic substrate can be transformed into commodity chemicals through photo- and electrocatalysis. He received his PhD in chemistry at Michigan State University, and then completed his postdoctoral study at Yale University. He is currently working on exploring different electrode materials to degrade organic refractory pollutants in water. Outside of lab work, Dr. Lam is also an educator and an environment enthusiast. During his postdoc appointment, he was invited to design and teach a green chemistry and sustainability certificate program at The University of Washington's Continuing Education Programs. After that, he became a visiting assistant professor at Wesleyan University before joining CityU.

TEACHING IRON TO PERFORM LIKE PALLADIUM IN CROSS COUPLING REACTIONS

Jordi Poater, Trevor Hamlin, F. Matthias Bickelhaupt and Xiaobo Sun

Departament de Química Inorgànica i Orgànica and Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona and ICREA, Spain

Abstract

We aim at developing design principles, based on quantum chemical analyses, for a novel type of iron-based catalysts that mimic the behavior of their well-known palladium analogs in the bond activation step of cross coupling reactions. To this end, we have systematically explored C–X bond activation via oxidative addition of CH_3X substrates (X = H, Cl, CH_3) to model catalysts $mFe(CO)_4q$ (q = 0, −2; m = singlet, triplet) and, for comparison, $Pd(PH_3)_2$ and $Pd(CO)_2$, using relativistic density functional theory at the ZORA-OPBE/TZ2P level. We find that the neutral singlet iron catalyst $1Fe(CO)_4$ activates all three C–X bonds via barriers that are lower than those for $Pd(PH_3)_2$ and $Pd(CO)_2$. This is a direct consequence of the capability of the iron complex to engage not only in π-backdonation, but also in comparably strong σ-donation. Interestingly, whereas the palladium complexes favor C–Cl activation, $1Fe(CO)_4$ shows a strong preference for activating the C–H bond, with a barrier as low as 10.4 kcal mol^{-1}. Our results suggest a high potential for iron to feature in palladium-type cross-coupling reactions.[1]

Biography

Jordi Poater got his PhD in Chemistry in 2003 at the Universitat de Girona (UdG) with a thesis on the analysis of chemical bonding and aromaticity of organic systems with tools based on the electron-pair density. Next he moved to the Vrije Universiteit Amsterdam (VUA), where he carried out research on the DNA replication mechanism by means of Kohn-Sham molecular orbital theory complemented with quantitative bond energy decomposition analyses. In 2016, Jordi was appointed ICREA Research Professor at the Universitat de Barcelona. He has published more tan 150 scientific publications in peer-reviewed journals, which have received more than 5.700 citations.

INFLUENCE OF HETEROCYCLIC LIGANDS ON CATALYTIC PROPERTIES OF OXOVANADIUM(IV) COMPLEX COMPOUNDS IN OLEFIN OLIGOMERIZATION

Joanna Drzeżdżon and Dagmara Jacewicz

Faculty of Chemistry, University of Gdansk, Poland

Abstract

Background: Polyolefins are used in many areas of life, e.g., polyethylene is used for the production of all kinds of packaging and tanks. One of the methods of obtaining polyolefins is polymerization with the use of metallocene and post-metallocene catalysts. Complexes which belong to post-metallocene catalysts are known as the precatalysts for olefin polymerization. Nowadays still looking for a new, more efficient catalysts.

Objective: To examine the influence of heterocyclic ligands on catalytic properties of oxovanadium (IV) complex compounds in olefin oligomerization.

Methods: The dipicolinate oxidovanadium (IV) complexes with 1,10-phenantroline and 2,2’-bipyridine have been tested towards their prediction of catalytic activities in oligomerization reactions of 2-chloro-2-propen-1-ol and 3-buten-2-ol. The series of oxovanadium (IV) complexes has been characterized by potentiometric method, NMR, IR, MALDI-TOF-MS. These complexes have been investigated as precatalysts after their activation by modified methylaluminoxane (MMAO-12). The oligomerization process has been conducted at nitrogen atmosphere, atmospheric pressure and at two temperatures: room temperature and 65 °C. The oligomerization products have been studied by several methods: NMR, MALDI-TOF-MS, TG, IR.

Results: The influence of heterocyclic ligands i.e., 1,10-phenantroline and 2,2’-bipyridine on catalytic properties of oxovanadium (IV) complex compounds in olefin oligomerization has been identified. The presence of a different type of ligand affects the catalytic activity, which in the case of oligomerization of 2-chloro-2-propen-1-ol hovers around 200 $g\cdot mmol^{-1}\cdot h^{-1}\cdot bar^{-1}$. While in the case of 3-buten-2-ol oligomerization the catalytic activities occurs on the level 1500 $g\cdot mmol^{-1}\cdot h^{-1}\cdot bar^{-1}$. Additionally, there are also noticeable differences in the structure and chain length distribution of the obtained oligomerization products.

Conclusion: The more basic heterocyclic ligand present in the coordination sphere of the catalyst metal ion, the higher the catalytic activity of the new precatalyst in the oligomerization reactions of 3-buten-2-ol and 2-chloro-2-propen-1-ol.

Biography

Joanna Drzeżdżon has her expertise in the synthesis new catalysts, studies on their physicochemical properties, as well as the using of chromium (III), vanadium (IV) and cobalt (II) complex compounds as olefin polymerization catalysts. She is a co-author of 45 scientific publications in international journals, as well as 2 patent applications. She is an employee of the Department of Environmental Technology, Faculty of Chemistry, University of Gdansk. She graduated in Chemistry at the Faculty of Chemistry of the University of Gdansk in 2012, where she also received a doctoral degree in 2017.

SUPERCRITICAL WATER GASIFICATION WITH LIGNOCELLULOSIC BIOMASS WASTE AS THE FEEDSTOCKS - ECONOMIC ANALYSIS OF NONCATALYTIC SCWG AT 600°C VERSUS CATALYTIC SCWG AT 400°C

Chai Siah Lee[1,2], Alex V. Conradie[2], Edward Lester[1]

[1]*Advanced Materials Research Group, University of Nottingham, United Kingdom*
[2]*Sustainable Process Technologies Research Group, University of Nottingham, United Kingdom*

Abstract

Background: Supercritical water gasification (SCWG) is a combined thermal decomposition and hydrolysis process for converting wet biomass feedstock to syngas rich in hydrogen. Noncatalytic SCWG are usually conducted at high temperature (e.g. ≥600°C) which leads to high capital and operating expenditure (CAPEX and OPEX). Heterogeneous catalysts (e.g. Nickel-based with metal oxide) have been tested in SCWG of biomass waste to enhance hydrogen yield whilst lowering reaction temperature to about 40 °C. However, economic analysis comparison between noncatalytic and catalytic SCWG with biomass waste feedstock has not been reported so far.

Objective: To conduct an economic study on the continuous-mode SCWG process with wheat straw as a feedstock to compare the CAPEX and OPEX of catalytic SCWG at 400°C with Ni/MgO as the catalyst and non-catalytic SCWG at 600°C and 22.1 MPa.

Methods: The SCWG model was developed by using Aspen Plus V11. Biomass was initially defined as non-conventional solid and the RYield block with FORTRAN subroutine was used to convert the solid biomass into its compositional elements, and then the RGIBBS reactor was used to predict the equilibrium product composition (H_2, CH_4, CO, CO_2, H_2O and ash) by applying direct minimization of Gibbs free energy.

Results: The results demonstrates that the catalytic SCWG at 400°C is theoretically more economically feasible than non-catalytic SCWG at 600°C due to the requirements of lower utility cost, CAPEX and OPEX at 400°C. Operation at 600°C requires the selection of high-grade heat-resistant and anti-corrosive fittings (e.g. Inconel 625) which is more costly when compared to lower temperature fittings (e.g. SS316).

Conclusion: The development of an eco-friendly catalyst that can reduce reaction temperature to 400 °C without compromising gasification efficiency and without losing its stability during continuous operation is highly important to accelerate the development of SCWG technology.

Biography

My current research focuses on supercritical water gasification (SCWG) for the production of green hydrogen. I work on the development and design of a highly efficient SCWG system as well as looking at how to optimise the whole process in order to reduce energy consumption, maximize the hydrogen yield and minimize the char formation that can cause blocking problems. I focus on using lignocellulosic biomass waste and wastewater from food and beverage industries as the feedstock of SCWG process. I also investigate feedstock pre-treatment methods before the SCWG process starts which can help to enhance biomass slurry pumpability during a continuous run, increase the biomass decomposition rate during gasification process that can lead to the improvement of gasification efficiency and hydrogen yield.

ROSEMARY ESSENTIAL OILS AS A PROMISING SOURCE OF BIOACTIVE COMPOUNDS: CHEMICALPROFILE, BIOLOGICAL ACTIVITY, THERMAL PROPERTIES, AND POSSIBILITY OF UTILIZATION AS ANTIOXIDANT AGENT

Saša Đurović, Pavel Riabov, Darko Micić, Rade Božović, Dušan Jovanović, Olja Šovljanski, Stevan Blagojević

Institute of General and Physical Chemistry, Serbia

Abstract

Background: Rosemary (*Rosmarinus officinalis* L.) is a worldwide cultivated plant mainly for essential oils, extracts, and as a spice. Up-to-date results showed diversity in composition of the essential oils, which may influence their quality, biological activity, and thermal properties. These differences are consequences of different geographical origin, seasonality, environmental condition, and varieties in rosemary.

Objective: to investigate the impact of geographical origin on the chemical composition, antimicrobial activity, and thermal properties of the rosemary essential oils originate from Serbia and Russia.

Methods: Serbian and Russian rosemary's essential oil were analyzed for chemical profile by the gas chromatography coupled with the mass spectrometry (GC/MS). Thermal properties were investigated by differential scanning calorimetry (DSC). Additionally, biological activity was assessed by using four bacteria strains, one yeast, and one fungi strain. After the initial assessment, essential oils samples were added to the sunflower oil in different amount for investigation of the possibility of their application as antioxidant agent during the frying process. Frying process was simulated on the DSC at the isothermal conditions at 140 °C. Obtained results were collected and presented in this article together with the corresponding discussion, while the conclusions were drawn aftermath.

Results: Investigation of the influence geographical origin on the chemical profile of the rosemary oil showed that there were differences in both composition and in content of the identified compounds in analyzed samples. Although the same compounds were the most abundant one in bot oils (α-pinene, eucalyptol, and camphor), both oils had specifical compounds which could be detected in only one sample but not in other. Such diversity significantly influenced the properties of the oils. Russian oil showed significantly higher antimicrobial activity against all tested strains. On the other hand, when oils were injected into a sunflower oil, Serbian oil proved to be more potent as antioxidant agent, while RF did not affect the stability in minor concentrations, but decreased oxidative stability of sunflower oil in higher concentration.

Conclusion: The application of the essential oil would highly depend on the chemical composition. Therefore, the oils have to be properly investigated prior to decision of the field of application.

Biography

Dr. Saša Đurović has gained his PhD in 2019 by defending the thesis titled „Contemporary methods of stinging nettle (Urtica dioica L.) extractions, composition and application of extracts". During his carrier as a researcher, Dr. Saša Đurović published 34 articles in SCI journals and four chapters. His areas of expertise are application of gas chromatography coupled with the mass spectrometry for analysis of different samples' types, application of both conventional and nonconventional extraction techniques for isolation of active compounds from plants, optimization of the extraction process, investigation of biological activity of prepared extracts, and their application in formulation of the new products.

ARTIFICIAL METALLOENZYMES BASED ON VANCOMYCIN FOR STEREOSELECTIVE CATALYSIS IN AQUEOUS MEDIA

Facchetti Giorgio, Isabella Rimoldi

University of Milan, Italy

Abstract

Background: Artificial metalloenzymes, stemming from the combination of transition metal catalysts embedded within a biological environment, have recently risen up as a promising approach to merge the reactivity of metal-based catalysis and the specificity of biocatalysis. Dalbapeptides, such as vancomycin, teicoplanin and ristocetin are variously substituted heptapeptides whose antibiotic activity depends on their binding to the D-Ala-D-Ala dimer of peptidoglycan precursors thus resulting in the inhibition of cell wall biosynthesis. In this system, indeed, the source of chirality is due to the presence not only of the aminoacidic chain, but also from the atropoisomerism of their structure. This interaction is stabilized by an array of hydrophobic interactions and five key hydrogen bonds and it is marked by such a low dissociation constant (KD = $\sim 10^{-17}$ M).

Objective: starting from this background, dalbapeptides can be employed as an innovative alternative to the classical biotin/(strept)avidin second sphere coordination system.

Methods: In this context, aminoethylbenzensulfonamide ligands decorated with the D-Ala-D-Ala dimer at different positions of the phenyl ring were employed for the synthesis of the hybrid catalysts in association with an iridium centre. In the presence of vancomycin, a new class of artificial reductases was obtained and applied to the stereoselective synthesis of chiral cyclic in different aqueous media.

Results: An encouraging 48% (S) e.e. was obtained in the asymmetric reduction of the salsolidine precursor in NaOAc 0.1 M buffer at pH 5 whereas in the case of the most demanding isoquinoline substrates, the meta-artificial metalloenzyme afforded the product in an outstanding 71% (S) e.e. when applied to quinaldine.

Conclusion: The Van/ D-Ala-D-Ala dimer system resulted particularly sensitive to pH variations, thus indicating an interesting change in the conformational arrangement of Van. Indeed, the system shows remarkable potential for the synthesis of chiral sultam precursors under green reaction conditions.

Biography

Giorgio Facchetti (35 publications, *h*-index 12) is actually a researcher fellow and Adjunct Professor of Organometallic Chemistry at the Department of Pharmaceutical Sciences, University of Milan. In 2015 he was awarded of the prestigious fellowship "Fondazione Confalonieri" soon after receiving his PhD in Chemical Sciences in 2014 at the University of Milan with a thesis entitled "New antiproliferative transition metal complexes: development and synthesis". His research interests deal with the synthesis of hybrid catalysts ("artificial metalloenzymes"), the design and synthesis of new chiral ligands for homogeneous catalysis and with antiproliferative platinum-based complexes.

A HIGHLY EFFICIENT TWO-STEP “GREEN” PROCESS FOR (-) AMBRAFURAN PRODUCTION

Lucia Steenkamp, Chris van der Westhuyzen, Kgama Mathiba

CSIR, South Africa

Abstract

Background: Ambergris, and more specifically its oxidation product (–)-ambrafuran, is a scarce, valuable and sought-after perfumery ingredient. The material is used as a fixative agent to stabilise perfumes in formulations by reducing the evaporation rate of volatile substances. Ambergris is a metabolic product of the sperm whale (*Physeter macrocephatus L.*), resulting from intestinal irritation.

Objective: To develop a green technology which is techno-economically viable for the production of (-) Ambrafuran.

Methods: Chemically, (–)-embrasure is produced from the natural product sclareol in eight synthetic steps – in the process using harsh and often toxic chemicals to do so. An overall yield of no more than 76% can be achieved in some routes, but generally this is lower. A new “green” route has been developed in our laboratory in which sclareol, extracted from the Clary sage plant, is converted to (–)-ambrafuran in two steps with an overall yield in excess of 80%. The first step uses a microorganism, *Hyphozyma roseoniger,* to bioconvert sclareol to an intermediate diol using substrate concentrations up to 50g/L.

Results: The yield varies between 90 and 67% depending on the substrate concentration used. The purity of the diol product is 95% and the diol is used without further purification in the next step. The intermediate diol is then cyclodehydrated to the final product (–)-ambrafuran using a zeolite, which is not harmful to the environment and is readily recycled. The yield of the product is 96% and following a single recrystallization, the purity of the product is >99.5%. A preliminary LC-MS study of the bioconversion identified several intermediates produced in the fermentation broth under oxygen- restricted conditions. Initially, a short-lived ketone is produced in equilibrium with a more stable pyranol, a key intermediate in the process. The latter is oxidised under Norrish type I cleavage conditions to yield an acetate, which is hydrolysed either chemically or under lipase action to afford the primary fermentation product, an intermediate diol. All the intermediates identified point to the likely CYP450 action as the key enzyme(s) in the mechanism.

Conclusion: This invention is an exceptional example of how the power of biocatalysis, combined with a mild, benign chemical step, can be deployed to replace a total chemical synthesis of a specific chiral antipode of a commercially relevant material.

Biography

Dr Lucia Steenkamp is a Principal Researcher at CSIR specialising in Biocatalysis and has been an author and co-author of numerous peer-reviewed papers and two book chapters. She has developed technologies for industry clients in the pharmaceutical, veterinary, biocides, food, flavours and fragrance industries, leading to five granted patents, nine technology demonstrators and five technology packages licensed to external clients. She has won the South African Women in Science Award (SAWISA) for Research and Innovation in 2018 for her work leading to technologies for commercialisation. She has been a finalist in the NSTF rewards in 2012, 2019 and 2020 for the development of new Green technologies.

PURPLE NON-SULFUR PHOTOSYNTHETIC BACTERIA AS A SOURCE OF BIOHYDROGEN AND BIOPLASTICS

Eleftherios Touloupakis

National Research Council, Italy

Abstract

Photosynthetic production of energy and organic materials addresses global warming and environmental pollution. Photosynthetic microorganisms, such as purple non-sulfur bacteria, are currently being investigated as potential sources of biomaterials and biofuels. The purple non-sulfur bacteria are fast-growing organisms, capable of achieving high biomass productivities and mainly use sunlight as the energy source. They are promising feedstock candidates for bioplastic, such as polyhydroxyalkanoates and biohydrogen (H_2) production. Polyhydroxyalkanoates are mainly accumulated in the cytoplasm of purple non-sulfur bacteria when they grow under stressful conditions. Purple non-sulfur bacteria produce biohydrogen by means of nitrogenase, using light as energy source and an organic substrate as an electron donor/a carbon source, in an anaerobic process called photofermentation. This work presents experimental results concerning purple non- sulfur bacteria growth in photobioreactors for the biohydrogen and poly-3-hydroxybutyrate production using synthetic culture broths and low-cost agro-industrial wastewaters. The results indicated the fact that cell growth, biohydrogen and poly-3-hydroxybutyrate production were affected by the type of carbon source in the culture broth.

Biography

Dr. Eleftherios Touloupakis is a permanent researcher at the Research Institute on Terrestrial Ecosystems of the National Research Council, Florence-Italy. He holds a doctorate and a master's degree in chemistry from the University of Crete-Greece. He has 20 years of laboratory experience in the fields of biochemistry and plant biotechnology. His research interest focuses on the development of technologies for the massive cultivation of photosynthetic microorganisms for applications in the renewable energy sector (biohydrogen) and bioplastics (polyhydroxyalkanoates). Author of 37 scientific publications, 4 book chapters and 1 patent.

PREPARATIVE REDOX TRANSFORMATIONS OF CARBONYL COMPOUNDS CATALYZED BY THE WHITE- ROT FUNGI

Tatyana Zhuk, Holger Zorn

Justus Liebig University Giessen, Germany
Igor Sikorsky Kyiv Polytechnic Institute, Ukraine

Abstract

Background: The relevance of biocatalytic approaches in organic synthesis is increasing, mainly due to the high selectivity, mild reaction conditions, and environmental safety of biocatalysis. Enzymes produced by white-rot fungi are among the most promising natural catalysts due to their ability to degrade robust biopolymers. Numerous studies of cell-free isolated fungal enzymes as well as of whole- cell systems have already been reported, however their preparative potential for selective transformations of organic compounds remains largely undisclosed.

Objective: Evaluation of the preparative potential of white-rot fungi for biotransformation of carbonyl compounds.

Methods: Biotransformations were performed with whole-cell growing cultures of white-rot fungi (*D. albidofuscus, D. squalens, M. cohortalis, P. sapidus, B. adusta*). To evaluate the chemical yields of the biotransformation reactions, a number of conversions were performed on preparative scale, and the resulting products were purified by column chromatography and analyzed by GC-MS, GC-MS-MS and NMR spectroscopy(Avance II 400 MHz WB and Avance III 600 MHz).

Results: The activity of the fungi was screened toward benzaldehyde, *p*-nitrobenzaldehyde, adamantanone and cyclohexanone, and the corresponding alcohols were obtained as products. *D. albidofuscus* was chosen for scaling up the reactions and preparative transformations. A number of substituted aromatic acids and aldehydes as well as saturated carbonyls could also be reduced with high preparative yields.

Conclusion: White-rot fungi display high selectivities in preparative bioreductions of aromatic acids and aldehydes. In case of saturated ketones oxidation of C–H bonds proceeds together with the reduction of carbonyl groups after 3 days of biotransformation.

Biography

With background in organic chemistry and technology Prof. Dr. Tatyana Zhuk actively works in synthetic organic chemistry, computational chemistry, surface chemistry, catalysis and publishes her results in world leading high impact journals (*J. Am. Chem. Soc., Org. Lett., J. Org. Chem., J. Phys. Chem.*, etc.). Currently she focuses on practical organic transformations in biocatalytic systems based on various fungi. She is interested not only in isolations of main reaction products but also in the mechanisms of biotransformations performing kinetic, isotope labeling studies, as well as isolation of pure enzymes for model experiments. She is an active lecturer and teaches students a number of basic and special courses in the field of organic chemistry and biochemistry.

LIVER-TARGETING CLASS I SELECTIVE HISTONE DEACETYLASE INHIBITORS POTENTLY SUPPRESS HEPATOCELLULAR TUMOR GROWTH AS STANDALONE AGENTS

Bocheng Wu[1], Subhasish Tapadar[1,2], Shaghayegh Fathi[1], Carrie Q. Sun[3], Idris Raji[1], Samuel G. Moore[1], Rebecca S. Arnold[3], David A. Gaul[2], John A. Petros[3] and Adegboyega K. Oyelere[1,2,4]

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Abstract

Dysfunction of epigenetic regulation in tumor is one of the driven force for tumor growth in multiple types of cancers. The balance between the two essential epigenetic enzymes Histone Deacetylase (HDAC) and Histone Acetyltransferase (HAT) can be altered, such that the HDAC activity may overregulate and silence major tumor suppressors. HDAC inhibition has been a promising anti-cancer therapy since 2005. To date, five HDACi were approved for lymphoma treatments. However, HDACi encountered with difficulties in solid tumor accumulation and lack of tissue-selective distribution with unclear reason. Hepatocellular carcinoma (HCC) is the most common type of liver cancer which is the fourth most common cause of cancer death in 2020 globally.[1] HCC is found to be highly regulating in HDAC isoform I (HDAC1, 2, 3) to control invasiveness and proliferation. Inhibition of HDAC class I could effectively suppress tumor growth and increase patient survival time. In this talk, we will unravel a liver-targeting HDACi with HDAC class I selectivity. This novel compound revealed selective HDAC 1 and 2 inhibition, while not valid for other HDACs. In cell cytotoxicity test, we found that the HCC cell lines are more sensitive to this candidate while the normal liver phagocytic cell Kupffer is not sensitive. In mice efficacy test, the candidate showed apparent liver accumulation and tumor suppression with no observable toxicity to mice. In addition, we observed that the compound is capable to penetrate the solid tumor. In such solution, we claim that this novel compound could have potential value in future drug development for HCC treatment.

1. Organization WH. Estimated Age-Standardized Incidence Rates (World) in 2020, All cancers, Both Sexes, All Ages. 2020.

SWELLING KINETICS AND THERMAL PROPERTIES OF HYDROGELS COMPOSED OF N-BUTYL ACRYLATE AND ISOBORNYL ACRYLATE

Ahlam Benkhelifa, Kamel Eddine Boudraa and Tewfik Bouchaour

University abou bekr belkaid Tlemcen, Algeria

Abstract

Background: An Interpenetrating Polymer Network, IPN, known as a blend of at least two polymers in a network form; One of them is synthesized and/or cross-linked in the immediate presence of the other(s). The synthesis of this new material class makes it possible to have in certain cases new materials with good performances in comparison with the initial polymer precursors.

Objective: In this work, we present a new sequential interpenetrating polymer network based on n-butyl acrylate (n-Abu) and isobornyl acrylate (IBoA), using a difunctional cross-linker 1,6-hexanedioldiacrylate (HDDA) and 2-Hydroxy-2-methyl-1-phenylpropane-1 (Darocur 1173) to initiate the radical polymerization under UV radiations.

Methods: The swelling kinetics of the polymer network was measured as function of the time at room temperature. The differential scanning calorimetry techniques allowed us to determine the thermal properties of the networks.

Conclusion: It is evident that the thermal properties of the IPNs are mainly influenced by the quantity of the monomer present in the polymer networks .This last does not present any phase separation.

Biography

Ahlam Benkhelifa is a PhD student in materials physic and composites, Researcher-students at the Macromolecules Laboratory at the University of Tlemcen in Algeria. Holder of a master's degree in polymer physics, my research focuses on the development and characterization of thermal and mechanical properties of polymers networks.

Day 2
Keynote

CURCUMIN AS A NOVEL REDUCING AND STABILIZING AGENT FOR THE GREEN SYNTHESIS OF METALLIC NANOPARTICLES FOR THEIR CATALYTIC APPLICATIONS

Digambara Patra

American University of Beirut Lebanon

Abstract

Curcumin is widely used in food, industries, cosmetic domain and in the biomedical field. It is obtained from food spices, turmeric, and clinically well known for its non-toxic and safe profile. The combination of green synthesis and curcumin to produce nanoparticles has been effective as the amount of toxic waste is highly reduced. Starting with a general introduction about nanoparticles synthesis and curcumin, the use of curcumin as a principal reducing agent and stabilizing compounds in the production of nanoparticles is developed. Consecutively, the preparation of different nanoparticles as gold nanoparticles (Au NPs), Silver nanoparticles (Ag NPs) and Copper oxide nanoparticles (CuO NPs) using curcumin has been investigated. For their applications, curcumin conjugated Au nanowires serve as excellent nano-catalyst for the reduction of nitro-compound and the rate of reduction of 4-nitrophenol by curcumin conjugated Au NWs is found to be ~10 fold higher than Au NPs, which signifies catalytic activities can be tuned by dictating size and shape of Au NPs. However, in case of curcumin conjugated Ag NPs it is found that smaller particles have better catalytic properties for the reduction reaction. On the other hand, the synthesized curcumin conjugated copper oxide nanograins are efficient nano-catalysts for the reduction of methylene blue and nanograin has better catalytic activity compared to spherical shape nanoparticles, emphasizing shape of the CuO particles is crucial for its nanocatalytic activity.

TAILORING DIFFUSIVE PATHWAYS AND THERMAL EXPANSION IN TI-ALLOYS

Matthias Bönisch

KU Leuven Kasteelpark, Belgium

Abstract

Ti-alloys are key materials in aerospace and biomedical engineering. Central for the optimization of their mechanical and functional behavior is in-depth knowledge on the complex interplay between diffusive and displacive phase transformations. Recently, 2 intriguing discoveries in relation to orthorhombic α″ phases in β-stabilized Ti-alloys were made: (i) the diffusion-controlled formation of α''_{iso} , α''_{lean} and α''_{rich} phases and ii) the giant and highly anisotropic thermal expansion of martensitic α″. Insight into both phenomena is limited, however needed for the tailoring of (micro)structures across a wide spectrum of configurations.

To address this challenge, I will demonstrate that the thermodynamic energy landscape reveals formation pathways for the diffusional forms of α″ and may lead to a stable β-phase miscibility gap in the binary Ti-Nb alloys. In this way, temperature-composition criteria for the occurrence of α''^{iso} and resolve reaction sequences during thermal cycling are derived. Further, I will revisit the giant (linear) thermal expansion in Ti-Nb alloys and will discuss processing routes to obtain null linear expansion in Ti-alloys. The presented concepts are expected to be transferable to other Ti-alloys and to catalyze new avenues for their tailoring and technological exploitation.

Biography

Matthias obtained his PhD degree in 2016 from TU Dresden, Germany, studying martensitic Ti-Nb alloys, their formation, mechanical behavior and thermal stability. Using *in-situ* high-energy X-ray diffraction (XRD) he discovered unusually large thermal expansion in Nb-rich martensite, the largest ever reported for a solid material to date. 2017 he spent as postdoc at University of Illinois at Urbana-Champaign, USA, investigating hardening mechanisms in high-entropy-alloys. In 2018 he joined KU Leuven (Belgium). In his current project, he links *in-situ* 3DXRD with crystal plasticity modelling. Matthias has (co-)authored 29 journal articles in reputed journals including Nature Communications.

PHOTOELECTROCHEMICAL REDUCTION OF N_2 TO NH_3 UNDER AMBIENT CONDITIONS THROUGH HIERARCHICAL $MOSE_2$@G-C_3N_4 HETEROJUNCTIONS

Muhammad Asim Mushtaq, Muhammad Arif, Xiaoyu Fang,Ghulam Yasin, Wen Ye,Majid Basharat, Bo Zhou, Shiyu Yang, Shengfu Ji and Dongpeng Yan

Beijing University of Chemical Technology, China

Abstract

Ammonia is a main precursor for the production of fertilizers, hydrogen energy carrier and emerging clean fuel that plays a crucial role in sustaining life on the globe. Nitrogen reduction reaction (NRR) based on photoelectrochemical (PEC) process is considered as an impending approach to achieve NH_3 production. Herein, hybrid $MoSe_2$@g-C_3N_4 micro/nanostructures are described that can serve as PEC catalysts to fix N_2 into NH_3 in basic electrolyte (0.1 M KOH) at low potential (−0.3 V *vs*. RHE) under ambient conditions. *In-situ* functionalization of the hierarchical micro/nanoflowers of $MoSe_2$ with exfoliated g-C_3N_4 nanosheets dramatically boost Faradaic efficiency and NH_3 yield rate up to 28.91% and 7.72 $\mu mol\ h^{-1}\ cm^{-2}$ respectively, which are higher than most of state-of-the-art NRR (photo)electrocatalysts. The high PEC activity can be attributed to the hierarchical architecture, light-harvesting capability, tunable active sites and formation of heterojunctions at the $MoSe_2$ and g-C_3N_4 interfaces, as confirmed by both experiments (PL, OCVD, EIS and UV–vis) and density functional theory (DFT) calculation. Therefore, this work not only develops an effective procedure to obtain hierarchical heterojunction catalysts towards robust and high-efficiency NRR based on PEC fashion, but also provides a deep understanding on the artificial N_2 fixation at the $MoSe_2$@g-C_3N_4 interfaces.

Scheme 1. Schematic representation for the fabrication procedure of hierarchical micro/nanoflowers of $MoSe_2$@g-C_3N_4 heterojunctions, (b) PEC performance of hierarchical micro/nanoflowers of $MoSe_2$@g-C_3N_4 heterojunctions.

COMPOSITE NANOFIBERS FOR IMPROVED PHOTOCATALYTIC PERFORMANCE UNDER UV AND VISIBLE LIGHT IRRADIATION

Mirela Suchea[1,2] and Petronela Pascariu[3], Emmanuel Koudoumas[1]

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Abstract

Background: One of the main problems of our day's research is environmental protection, especially the purification of wastewater and air that has caused globally alarming concern. Many studies have been based on the development of new oxide semiconductor materials with improved photocatalytic activity under UV or sunlight irradiation, for both wastewater treatment and air pollution. Water purification has become an intensely analyzed topic for the scientific world. Besides other contaminants, organic dyes, represent between 10 and 15% of pollutants that reach groundwater during industrial processes.

Objective: The main objective of this study is the development by electrospinning-calcination method of new TiO_2 based photocatalyst materials, Metal and metal oxide/TiO_2 nanocomposites with different compositions targeting remarkable photocatalytic performance, easiness to recover and an excellent activity under UV and visible light irradiation.

Methods: Fabrication of new TiO_2 based photocatalyst materials by electrospinning-calcination method. Typical characterization of the fabricated nanocomposites was performed using the X-ray diffraction (XRD), scanning electron microscopy (SEM), FT-IR, Raman spectroscopy, ultraviolet–visible spectroscopy (UV–vis).

Results and Conclusion: TiO_2 based nanocomposite photocatalytic fibrous materials fabricated by electrospinning-calcination method. Various compositions TiO_2 based nanofibers with various physical properties were obtained. Crystallinity of the TiO_2 based materials can be tuned by controlling the temperature of calcination. By calcination temperature control, fibers in all crystalline TiO_2 phases can be easily obtained using a simple and scalable fabrication technique. The nanocomposite fibers with diameters between 50 nm and 150 nm can be easy fabricated for obtaining photocatalysts immobilized onto substrates or embedded in polymeric matrices to reduce the environmental contamination risks. For the case of materials produced during this study the risks are much lower and they provide an easy recovery from their duty site. All the studied materials show physical properties that make them suitable for UV and visible light photocatalyst applications and many other environmental, health, electronic and optoelectronic applications.

Biography

Mirela Suchea is affiliated to CEMATEP, Hellenic Mediterranean University, Heraklion, Greece and National Institute for R&D in Microtechnologies - IMT Bucharest, Romania. She is a scientist with research experience in the field of nanostructured materials synthesis and applications. She works in materials science and nanotechnology since 2002, being author and coauthor of more than 60 journal articles (over 1100 citations), and books chapters in a broaden interdisciplinarity between nanotechnology, materials science, physics, chemistry, electrochemistry.

TYPHA ANGUSTIFOLIA, A BENEFICIAL PLANT FOR WASTEWATER TREATMENT

I.C. Covaliu, L.I. Diaconu, I.R. Suica-Bunghez, G. Paraschiv

Polytechnic University of Bucharest, Romania

Abstract

Background: In the last years, wastewater contains many pollutants because of the industries production. There are different kinds of pollutants like pesticides, insecticides or heavy metals.

Objective: In this research, we focused on heavy metals (Mangan) which are a toxic pollutant.

Methods: The experiment consisted of immersing three *Typha angustifolia* plants in a volume of wastewater (2,5 L), contaminated with Mn II (2 mg/L), at different times (8, 16, 24 ,32, 40 h), homogenizing the fluid using a magnetic stirrer. It was used a WTW Photolab S12 colorimeter.

Results: It was observed that the three rush (*Typha angustifolia*) plants had the retention capacity of Mn (II) ions in the 3 rush plants, gradually increases with the increase of the time period, of contact of the plants with the wastewater. At the same time, it is observed that the yield increases with the increase of the contact time between plants and Mn (II) ions, at 8 hours, the yield being only 30%, and the yield obtained after 40 hours increased reaching a maximum of 77.5% ability to retain Mn (II) ions gradually, as the time period increased in wastewater.

Conclusion: It has been observed that aquatic plants can be used in water purification. *Typha angustifolia* was found to have a yield of 77.5%, in retaining Mn (II) ions, this capacity being obtained due to the number of plants applied in the experiment, but also by the type of pollutant (manganese, in the case of this study).

Biography

I.C. Covalu is a professor at the Faculty of Biotechnical Systems Engineering, POLITEHNICA University of Bucharest, she completed her postdoctoral fellowship in 2013, her doctorate in 2010, her master's degree in 2008 and her bachelor's degree in 2006. She has over 10 years of experience in obtaining and characterizing nanomaterials, competences in FTIR, UV-VIS, ISI articles over 45 and numerous national and international conferences.

BIOCATALYTIC APPROACH FOR DIRECT ESTERIFICATION OF IBUPROFEN WITH SORBITOL IN BIPHASIC MEDIA

Federico Zappaterra, Daniela Summa, Bruno Semeraro, Stefania Costa and Elena Tamburini

University of Ferrara, Italy

Abstract

Background: Ibuprofen is a nonsteroidal anti-inflammatory drug (NSAID) introduced in the 1960s and widely used as an analgesic, anti-inflammatory, and antipyretic. In its acid form, the solubility of 21 mg/L greatly limits its bioavailability.

Objective: Since the bioavailability of a drug product plays a critical role in the design of oral administration dosage, this study investigated the enzymatic esterification of ibuprofen as a strategy for hydrophilization. This work proposes an enzymatic strategy for the covalent attack of highly hydrophilic molecules using acidic functions of commercially available bioactive compounds.

Methods: The poorly water-soluble drug ibuprofen was esterified in a hexane/water biphasic system by direct esterification with sorbitol using the cheap biocatalyst porcine pancreas lipase (PPL).

Results: The optimization of the biocatalytic biphasic process, such as lipase and compounds concentrations, solvents amount, temperatures, stirring speed, and times is reported.

Conclusion: PPL demonstrated itself to be a suitable enzyme for the effective production of the IBU-sorbitol ester. This is the first time that enzymatic esterification of IBU-sorbitol ester has been proposed.

Biography

Dr. Federico Zappaterra is a molecular biologist who is undertaking a Ph.D. in biomedical and biotechnological sciences; His work concerns the development of enzymatic modification protocols for poorly bioavailable active ingredients of pharmaceutical and agri-food interest. His expertise deals with free and immobilized enzymes for the esterification of active compounds using a green eco-sustainable approach. Federico's work focused on the study of the non-steroidal anti-inflammatory drug Ibuprofen, the third most prescribed drug in the world. The innovative protocols he developed, some of them patented, allowed him to design six derivatives of ibuprofen enhanced in water-solubility.

COMPOSITE CORE@SHELL MICROGEL PARTICLES FOR CATALYTIC REDUCTION OF TOXIC NITROARENES

Khalida Naseem

University of Central Punjab, Pakistan

Abstract

Various toxic dyes and nitro-aromatic compounds are present in industrial effluents. These effluents are exposed to water sources and cause serious issues to environment and living organisms. Therefore, removal/degradation of these toxic pollutants from wastewater sources is need of time. Here, silver nanoparticles fabricated polystyrene-poly(N-isopropyl methacrylamide-acrylic acid) core shell particles were prepared in three steps via precipitation polymerization, seed mediated emulsion polymerization and *in-situ* chemical reduction methods. These prepared composite particles were used as catalyst to degrade toxic dyes such as Congo red (CR), Rhodamine B (RhB) and Methylene blue (Mb) and various other nitroaromatic compounds like 4-Nitrophenol (4-NP) and 4-Nitroaniline (4-NA) in presence of sodium borohydride ($NaBH_4$) as reducing agent. Controlled reactions were also performed to prove high activity of core@shell composite. Value of rate constant for degradation of toxic pollutants was evaluated by adopting pseudo first order kinetic model. Dyes reduction reactions were evaluated on the basis of Langmuir Hinshelwood (L-H) mechanism. Pollutants degradation was also performed under different reaction conditions such as catalyst dose, NaBH4 and amount of toxic dye to maximize the potential of catalyst. Nano-catalyst exhibits high activity upon repeated recycling.

Biography

Dr. Khalida Naseem obtained her Doctorate degree in Chemistry from Institute of Chemistry, University of the Punjab, Lahore in September 2019. She served as Lecturer in Kinnaird College for Women, University of the Punjab and Minhaj University, Lahore, Pakistan. She also worked in University of the Punjab as research officer for two years. She is currently serving as Assistant Professor in Faculty of Sciences, University of Central Punjab, Lahore. She has published 38 articles in journals of international repute with an accumulative impact factor of 131.09. She presented her research work as poster/oral presenter in various National and International conferences. Dr. Khalida Naseem is a member of the Chemical Society of Pakistan and American Institute of Chemical Engineering, USA.

TOWARDS AN IDEOTYPE FOR FOOD-FUEL DUAL-PURPOSE WHEAT IN ARGENTINA

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Universidad Nacional de Mar del Plata, Balcarce, Argentina

Abstract

Background: Wheat straw (*Triticum aestivum L.*) is one of the most abundant agricultural residues worldwide. It can be used to produce biogas, one of the most efficiently produced renewable energies. Wheat grown with the dual purpose of producing food and biogas should display simultaneously high grain and straw yields, low lodging susceptibility and high conversion efficiency of straw into biogas[4].

Objective: The aims of this study were to determine the best food-fuel dual-purpose wheat candidates among wheat genotypes used in breeding programs in Argentina and to gain some insights into the relationships between key traits relevant for dual-purpose genotypes.

Methods: Grain (GY) and straw (SY) yields were determined in 36 genotypes of wheat —including French, CIMMYT and local (Criollo) germplasm— during 2014 and 2017. Lodging susceptibility (LS) was determined following Mirabella et al. (2019). Straw conversion into biogas was measured in terms of biogas potential production and kinetic parameters Bmax (maximum specific biogas production) and k (first-order kinetic constant). Key traits were together analyzed by a principal component analysis. Percentile-based thresholds were used to identify candidate genotypes.

Results: High variability GY, SY, LS, B_{max} and k has been found. Baguette 31 and SNR Nogal, two genotypes of French origin, showed high GY and SY, low LS, and moderate-to-high B_{max} and *k*. Buck Guapo and Buck Baqueano, two genotypes of Criollo origin, displayed good values GY, SY and Bmax and k. However, their high LS precludes their production in shallow soils or high-input systems. Some old genotypes (e.g. Klein Atlas) harbored a good combination of all key traits and could prove valuable to be included in future breeding programs for dual-purpose wheat.

Conclusion: While none of the genotypes excelled in every key trait, a few candidates showed potential for dual-purpose ideotype. The challenge lays in gathering all attributes for food and 2G fuel in the same genotype

Biography

Dr. Mercedes Echarte is a scientific researcher from the National Institute of Agricultural Technology and the National Scientific and Technical Research Council (Argentina). She is a Biochemist (PhD), Project Leader and Head of the Biomass and Bioenergy Laboratory (IPADS, INTA-CONICET). She has been long working on plant physiology, biomass production and bioenergy. One of her current scopes of her Lab is to foster the role of agriculture in the energy sector by designing strategies for sustainable bioenergy production. Since 2015 she has also been running a transformative science experience, where knowledge generated in the academic sector is used to transform a society into a more sustainable one: "Biogas demonstration unit for a sustainable rural energy development in humid Pampas of Argentina".

BIOLOGICALLY PLANT-BASED PIGMENTS IN SUSTAINABLE INNOVATIONS FOR FUNCTIONAL TEXTILES – THE ROLE OF GREEN CHEMISTRY

Alka Madhukar Thakker

Heriot - Watt University, UK

Abstract

The textile industry is witnessing a paradigm shift towards sustainability to circumvent ecological dilemmas and human health jeopardies arising from textile processing. Therefore, the review paper herein focuses on the role of green chemistry in synthesizing the natural biological pigments and bio-mordants for textile substrates such as Sarsasapogenin and soyasaponin from areetha nut extract. Concurrently, the overview aligns the data on the chemical characterization of these plant-based renewable pigments for textile processing that is chlorophyll, carotenoids, flavonoids others. Likewise, the subtle and vital role of bioactive biological compounds in plant pigments for functional textiles applications for example antibacterial, analgesic, and more is succinctly accentuated. The review paper identifies the substantial surplus reserve of plant-based materials that could be conserved for sustainable implications in the textile field. However, there is a prodigious scope of research and development in the same and therefore concludes by citing the multi-disciplinary research as future work to mitigate declared climate emergency for international thriveability. Likewise, the responsibility of conserving biodiversity, adhering to sustainable development goals, and cradle to cradle theories are reinforced in the review paper.

REMOVAL PERSISTENT POLLUTANTS BY FENTON SYSTEMS: ENHANCING DEGRADATION BY BIO-BASED CHELATING AGENTS.

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[2]Universidad de Concepción, Chile

Abstract

Background: Water is a vital resource for all kind of life. However, today is frequent the detection of several contaminants on water supplies. Fenton processes have been widely studied by their application in water remediation. The use of ligands such as 1,2-dihydroxybenzenes (DHBs) is one of the alternatives to increase the oxidizing ability of these processes. As the oxidation efficiency can be restricted by the cycle reduction Fe^{3+}/Fe^{2+}, these chelating agents can influence these processes according to pH modulation, and the enhancement of reactivity by the iron complexation. The main issue of these ligands is the production of toxic quinones and their subsequent release to the environment. Consequently, a heterogeneous system, with DHBs held in a solid support, is proposed as a promising strategy to avoid this disadvantage. A renewable source of DHBs is *Pinus radiata* bark, specifically, condensed tannins, which are mainly monomeric units of catechin or epicatechin linked, with a B-ring available for iron complexation.

Objective: Water-insoluble tannins were used as a source of DHBs to promote the oxidizing ability of Fenton processes.

Methods: Optimization studies were performed in order to find the optimal conditions for degradation of pollutants. The activated species generated in these heterogeneous systems were determined by EPR, also the reactivity pathways and oxidation by-products by HPLC and GC-MS.

Results: The oxidizing ability of the developed heterogeneous Fenton systems was significantly increased in presence of insoluble tannins obtained from the *Pinus radiata* bark.

Conclusion: The heterogeneous Fenton using a biobased ligand has significantly higher efficiency to degrade atrazine and methylene blue than conventional processes. The repetitive use of the tannins showed similar oxidizing ability and not showed lixiviation of phenols or other aromatic compounds.

Acknowledgement: FONDAP Solar Energy Research Center ANID/FONDAP/15110019.

Biography

Dr. Romina Romero is Associate Researcher at Universidad de Tarapacá, and Postdoctoral Research Fellow by FONDAP/Solar Energy Research Center (SERC-Chile). She has a B.Sc. in Chemistry (2012) and a Ph.D. in Science and Analytical Technology (2016) from Universidad de Concepcion. She has participated in more than 15 indexed scientific publications, 3 book chapters, several international collaborations, 2 international internships, and more than 10 participations in R&D projects in the last 5 years. She has participated in human capital formation through thesis direction, internships, and teaching at undergraduate and graduate level. Her main research lines are associated to waste valorization, mainly biomass, and its application in oxidative systems for wastewater remediation. Also, the improvement in the degradation efficiency of oxidative systems by incorporation of biobased ligands and sunlight irradiation.

NOVEL GLYCOSYLATED HISTONE DEACETYLASE INHIBITORS FOR TARGETED TREATMENT OF HEPATOCELLULAR CARCINOMA

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[1]*Georgia Institute of Technology, USA*
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Abstract

Hepatocellular cancer (HCC) is a heterogeneous cancer sustained by gene-silencing chromatin histone hypoacetylation due to dysfunctions in the activities of histone deacetylases (HDACs).[1] HCC is also highly dependent on Warburg effect with overexpression of GLUT-2 transporter, an altered state of metabolism in which cancer cells depend on anaerobic glycolysis for energy source.[2] Herein we reported the integration of glycoside moieties into the prototypical HDAC inhibitors (HDACi) surface recognition group to afford glycosylated HDACi. Lead compound STR-V-53 intracellular on-target effects and displayed exquisite HCC cell line selectivity, as it is non-toxic to all 60 cell lines in the NCI-60 panel and derived a significant part of its Hep-G2 cell penetration through GLUT-2-mediated transport. Furthermore, STR-V-53 is relatively non-toxic to mice up to 50mg/kg dosage and robustly suppressed tumor growths in an orthotopic model of HCC as standalone agent. STR-V-53 also enhanced the potency of Sorafenib (SORA), an HCC standard of care, in a combination therapy experiment. Collectively, our data suggests that STR-V-53 is a novel HDACi whose potential as targeted anti-HCC agent merits further evaluation in additional preclinical studies.

Posters

CATALYTIC ACTIVITY OF PLASMA-PREPARED THIN FILMS BASED ON MIXED COBALT AND IRON OXIDES IN CO2 CONVERSION TO CO

Hanna Kierzkowska-Pawlak[1], Ryszard Kapica[1], Małgorzata Ryba[1], Maciej Fronczak[1], Jan Sielski[1], Bartłomiej Januszewicz[2], Jacek Tyczkowski[1]

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[2]*Institut of Materials Science and Engineering, Lodz University of Technology, Poland*

Abstract

Background: The hydrogenation of CO_2 to produce CO and H2O, known as reverse water gas shift reaction (RWGS) is considered an important CO_2 valorization pathway. A key challenge in designing efficient catalysts for this purpose is to improve the low-temperature performance and selectivity of the RWGS reaction, which competes with exothermic CO_2 methanation.

Objective: This work is aimed at proposing new plasma-prepared thin-film catalysts for RWGS reaction.

Methods: Novel nanocomposites based on mixed cobalt and iron oxides were prepared by the plasma-enhanced chemical vapor deposition (PECVD) from organic cobalt and iron precursors on a structured support in the form of a wire mesh. By controlling the relative flow rates of iron and cobalt precursors, various thin films with different Fe/(Fe+Co) atomic fractions were produced in a 60 W glow discharge RF plasma reactor and then calcined at 400°C under an argon flow. The catalysts were characterized by SEM/EDX, XPS and XRD techniques. The kinetic tests were performed in a tubular reactor in the range of 300–400°C under atmospheric pressure (H_2/CO_2=4:1, 25 sccm, m_{cat}=0.7 g).

Results: The films based on single CoO_X and FeO_X, as well as the series containing mixed oxides were stable and active in hydrogenation of CO_2. The CoO_X-based catalyst exhibited high activity towards methane, while the FeO_X-based catalyst was much less active and converted CO_2 mainly into CO (400^{o}C: XCO_2=10%, SCO=88%). A small fraction of iron in the Fe–Co nanocomposite inhibited the production of methane. On the other hand, with increasing Fe fraction in the nanocomposite, the efficiency of the RWGS reaction increased compared to pure FeO_X, reaching 95% selectivity to CO and approx. 30% conversion of CO_2 at Fe/(Fe+Co) = 0.6–0.8.

Conclusion: The plasma-prepared Fe–Co nanocomposites showed superior performance in the RWGS reaction compared to thin films based only on FeO_X.

Biography

Ryszard Kapica researches in the field of chemical engineering with particular emphasis on non-equilibrium plasma engineering, catalysis on materials produced and modified with plasma methods, and molecular engineering.

CATALYTICAL ACTIVITY OF TUNGSTEN-CONTAINING THIN FILMS DEPOSITED BY PLASMA ENHANCED CHEMICAL VAPOR DEPOSITION METHOD

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Abstract

Background: Tungsten-containing materials are well-known catalysts for a wide range of industrial applications such as Fisher-Tropsch synthesis, crude oil processing or the reduction of environmentally unfriendly gases, to mention the most important. An interesting compound is tungsten carbide. Its catalytic properties have been found to be similar to that of Pt. There are several methods of producing this type of materials, e.g., the pyrolysis of organometallic compounds or reactive sputtering. Plasma Enhanced Chemical Vapor Deposition (PECVD) is an attractive alternative for the production of thin-film catalysts with a controlled composition.

Objective: The aim of this work was to obtain tungsten-based thin films using the low-pressure PECVD process, in which W(CO)6 was used as a precursor. An important aspect of this work was also the analysis of catalytic activity in the CO_2 conversion reaction to synthetic gas.

Methods: The thin films were deposited on calcined Canthal steel at a temperature of not higher than 120°C, at pressure below 1.0 Pa with Ar as a carrier gas. The surface analysis of the as-deposited and post-process films was carried out by using X-ray photoelectron spectroscopy (XPS) and scanning electron microscopy (SEM) in terms of their molecular structure and microstructure. Additionally, X-ray diffraction (XRD) was performed to determine the phase composition. The catalytic behavior of the samples was tested in a tubular reactor at temperatures up to 600°C by means of gas chromatography (GC).

Results: Obtained thin films contained 15–25 at% of W in form of oxides and carbides with different proportions. The catalytic activity rise with temperature up to around 25% CO_2 conversion at 600°C.

Conclusion: The study shows that the chemical structure of the films differs depending on the used parameters of the plasma deposition. In the $CO_2 + H_2 \rightarrow CO + H_2O$ reaction all samples showed promising catalytic activity.

Biography

Aleksandra Kędzierska-Sar has her expertise in materials science, especially in nanomaterials synthesis and designing for different applications like biomaterials, high hardness – high toughness composites or lastly – thin-films for catalytic applications. She has in hands experience with wide range of analytical methods which enables the analysis of research results from a broad scientific perspective. From deep analysis of material structure and properties to finding a correlation between structure and application properties of designed material. A creative, open and optimistic person.

BIOLOGICALLY PLANT-BASED PIGMENTS IN SUSTAINABLE INNOVATIONS FOR FUNCTIONAL TEXTILES – THE ROLE OF BIOACTIVE PLANT PHYTOCHEMICALS

Alka Madhukar Thakker

Heriot - Watt University, UK

Abstract

The fossil-based emissions and effluents from the textile wet processing units have acute implications on the environment and human wellbeing. Therefore, a paradigm shift towards sustainable alternative materials and technology has become imperative. Thus, the overview herein emphasizes the sustainable chemistry that ubiquitously exists to propel ecological textile processing with herbal biomaterials. The review paper succinctly accentuates the efficient qualities of bioactive plant pigments for functional textiles. The paper also outlines the sustainable method of processing with plant phytochemicals. The eco-friendly herbal materials as an excellent example of Biomimicry is presented. Likewise, the multi-disciplinary research approach is discussed herein to refute global dilemmas and impel holistic ecological outcomes. The circular materials for the circular economy are detailed.

Video Presentations

SURFACTANT-FREE COLLOIDS: GREENER SYNTHESES FOR NANOPARTICLE AND NANOCATALYSTS

Jonathan Quinson

University of Copenhagen, Denmark

Abstract

Background: Nanomaterials (NMs) are key in a range of applications covering medicine, optics, energy conversion and chemical production. Nowadays, a range of methods allow to produce the required NMs with the required properties, for instance using colloidal syntheses. In order to obtain stable NMs by colloidal routes, surfactants are typically added. Unfortunately surfactants and other additives often block catalytically active sites of the NMs and so needs to be removed. Surfactants not only typically derived from fossil-fuels, but their removal before applications in catalysis or medicine, require time and energy consuming steps.

Objective: Over the last years, we have been developing surfactant-free syntheses of nanoparticles (NPs) to address the above mentioned challenges, in order to make the synthesis but also applications of NPs more sustainable. We focused on precious metal NPs used as catalysts for energy conversion.

Methods: The method to obtain the surfactant-free yet stable colloidal nanomaterials is simple, requires relatively safe chemicals and reactions conditions, e.g. relatively low temperatures, simple low boiling point mono-alcohols and water together with a base and a metal precursor.

Results: The nanoparticles obtained by this low boiling point surfactant-free colloidal synthesis strategy show a range of promising properties demonstrated for various reactions relevant for energy conversion for metals a diverse as platinum, iridium, palladium or gold.

Conclusion: A new and simple surfactant-free synthesis of precious metal nanoparticles is presented. The parameters that control the resulting properties of the nanoparticles such as size are described. The relevance of the materials obtain for various reactions relevant for energy conversion towards more sustainable energy supply is demonstrated.

Biography

Dr Jonathan Quinson studied at ESPCI ParisTech France (MSci, 2010) and Imperial College London, UK (MRes, 2011) before receiving his PhD from the University of Oxford, UK (2016). He is now a Marie-Skłodowska Curie Fellow affiliated with the University of Copenhagen, Denmark. His main research interests are the sustainable synthesis of nanomaterials with a focus on developing new and industrially relevant surfactant-free synthesis of colloidal nanomaterials for application in (electro)catalysis. He authored 43 publications on the synthesis and applications of nanomaterials and hold 1 patent. His broadest areas of interests are green chemistry, energy conversion and nanomaterials.

GREENHOUSE COVERING PLASTICS FILMS WASTE MANAGEMENT: A Case-Study GIS - BASED MODEL

Monica Parlato, Simona Porto and Francesca Valenti

University of Catania, Italy

Abstract

Background: In a circular economy framework, the conversion of waste into new raw material is an important aspect of increasing resource efficiency, by reducing environmental pollution and CO2 emission. One of the biggest environmental concerns is plastic pollution, a cause of the long-life material (plastic can take hundreds or thousands of years to be decomposed) and because more than 85% of plastic waste ends up in landfills or are wrongly disposed of.

In Europe, plastic material, especially plastic films, used in agricultural activities are more than 1 million tons per year. In the absence of a correct policy disposal of plastic films, environmental degradation takes place with serious consequences for air, water and landfill.

Objective: In this research, a geographical information system (GIS) - based model to locate and quantify the yearly amount of agricultural plastic waste (APW) coming from crop-shelter coverage used in greenhouses system was put forward and applied in a study area located in southern Italy, which is highly characterized by protected cultivation practices.

Methods: The areas with the highest density of crop shelters were mapped, then a suitable index to determine APW amount was computed and applied to obtain heat maps related to covering plastic films. Results: The computed average values of PWIG and PWIT were 1,477 kg $ha^{-1}yr^{-1}$ and 1,978 kg $ha^{-1}yr^{-1}$, respectively.

Conclusion: GIS-based model results could provide basic information for the analysis of the environmental impact due to APW supply. Therefore, these results could offer a suitable tool to improve the correct disposal management of covering plastic films and the related recycle policy.

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BOOKMARK YOUR CALENDAR

July	
Webinar on Dentistry and Oral Health	July 05-06, 2021
4th International Webinar on Nanotechnology & Nanomaterials	July 05-06, 2021
4th Webinar on 3D Printing & Additive Manufacturing	July 05-06, 2021
International Webinar on Graphene and Semiconductors	July 05-06, 2021
Online International Conference on Diabetes and Endocrinology	July 19-20, 2021
Webinar on Pediatrics and Neonatology	July 19-20, 2021
3rd Online International Conference On Nutrition and Nutraceuticals	July 19-20, 2021
International E-Conference on Gastroenterology and Hepatology	July 23-24, 2021
International E-Conference on Digestive and Metabolic Diseases	July 23-24, 2021
Webinar on Laser, Optics & Photonics	July 26-27, 2021
International Webinar on Quantum Physics and Nuclear Technology	July 26-27, 2021
International Webinar on Magnetism and Magnetic Materials	July 26-27, 2021
Online International Conference on Atmospheric and Earth Sciences	July 29-30, 2021
3rd Webinar on Plant Science & Molecular Biology	July 29-30, 2021
4th Webinar on Agriculture, Food & Aqua	July 29-30, 2021

August	
Online International Conference on Civil Engineering & Architecture Design	August 03-04, 2021
Webinar on Construction & Steel Structure	August 03-04, 2021
Webinar on Food Nutrition and Dietetics	August 05-06, 2021
International Webinar on Mass Spectrometry & Analytical Techniques	August 05-06, 2021
2nd E-Meeting on Polymer Science & Biomaterials	August 05-06, 2021
International Webinar on Artificial Intelligence and Robotics	August 11-12, 2021
Webinar on Remote Sensing and Geosciences	August 11-12, 2021
Webinar on Sensors and Actuator Networks	August 11-12, 2021
2nd Online International Conference on Microbiology	August 26-27, 2021

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BOOKMARK YOUR CALENDAR

September	
2nd International Webinar on Dentistry and Dental Materials	September 02-03, 2021
2nd International Webinar on Big Data Analytics & Data Science	September 06-07, 2021
3rd European congress on Material Science & Nanotechnology	September 16-17, 2021
2nd European Congress on Addiction, Psychiatry and Mental Health	September 16-17, 2021

BOOKMARK YOUR DATES

2nd Webinar on

BIOCATALYSIS & GREEN CHEMISTRY

November 04 - 05, 2021

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