

Environmental & Green Chemistry 2017



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

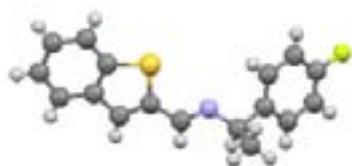
Posters

Environmental & Green Chemistry 2017

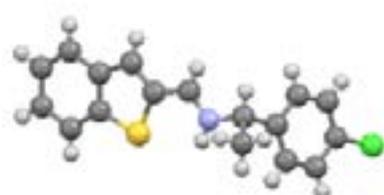
Green synthesis of new chiral halogenated imines derived from Benzo[b]thiophene-2-carboxaldehyde

Andrea Moreno Ceballos, Guadalupe Hernández, Gloria E Moreno, Oscar Portillo and René Gutiérrez
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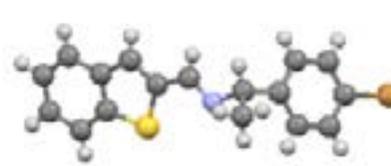
Pollution must be taken seriously, because it reduced large reserves of water in the world, and acid rain deteriorated the health of forests, etc. Some chemicals were suspected of causing these problems. Consequently, there have been different proposals on the design, development and implementation of chemicals. These proposals benefit the economy; protect the population and the planet, thus achieving a reduction of waste, conserving energy. In addition, it is important to consider the life cycle of the reagents from the time they are obtained to the final disposal of the reagents. Solvent-free organic synthesis has expansive prospects as well as many advantages such as high efficiency, easy separation and purification and environmental acceptability. All these merits are in accord with the Green Chemistry's requests of energy-saving, high efficiency and environmentally benign. Compounds containing an imine group are known to play an important role in living organisms, and some reports have established that the presence of imine or azomethine subunits in various natural, natural-derived, and non-natural compounds was critical to their biological activities. We are currently engaged in a program dedicated to the synthesis of small Schiff bases using a single-step solvent-free approach. We performed the preparation of three chiral imines 1, 2 and 3 derived from benzo[b]thiophene-2-carboxaldehyde and the optically active halogenated amines (S)-(-)-1-(4-fluorophenyl)ethylamine, (S)-(-)-1-(4-chlorophenyl)ethylamine and (S)-(-)-1-(4-bromophenyl)ethylamine, respectively in excellent yields.



Crystal structure of imine 1



Crystal structure of imine 2



Crystal structure of imine 3

Biography

Andrea Moreno pursued her Postgraduate studies with Master's in Organic Chemistry at the Faculty of Chemistry, Benemérita Universidad Autónoma de Puebla. She is passionate about the Green Chemistry, the development of environmentally improved routes, synthetic methods and processes to important products and the chemical aspects of renewable energy. Also, she is interested in the structural elucidation, green synthesis, X-ray crystallography, structure-NMR spectra relationship and mass spectrometry.

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Notes:

Green synthesis of chiral imines and their Zn(II) complexes

Daniela Gutiérrez, Eduardo Brambila, Alejandro Ruíz, Carolina Gutiérrez, Guadalupe Hernández, Gloria E Moreno, Oscar Portillo and René Gutiérrez
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Statement of the Problem: Nowadays, reactions conducted in the absence of solvents under mild reaction conditions are becoming an important method in laboratories worldwide as an environment-friendly technique for the efficient syntheses of organic molecules. The main advantages of solvent-free organic synthesis are shorter reaction times, minimum waste and generally higher yields, operational simplicity as well as reduction of thermal degradative byproducts along with cleaner work-up.

Methodology: The preparation of two chiral imines derived from 2-pyridylcarboxaldehyde and the optically active primary aromatic amine (S)-(-)-1-(4-methylphenyl) ethylamine and (S)-(-)-1-(4-methoxyphenyl) ethylamine by solvent-free techniques.

Findings: The ligands obtained were allowed to coordinate with Zn(II) also under solvent-free conditions affording complexes 1 and 2, respectively. The products were characterized by using spectroscopic techniques (FT-IR, NMR H and C, EI-MS) and the structure of the Zn(II) complexes was fully confirmed by X-ray diffraction studies. The antimicrobial activity of the complexes (I)–(III) was evaluated against Gram positive (*Staphylococcus aureus*) and Gram negative (*E. coli*, *Pseudomonas aeruginosa*) bacteria, and yeast (*Candida albicans*).

Conclusion & Significance: The complexes were found to possess noteworthy antimicrobial activity.



Figure: Crystal structure of complex 1 and Crystal structure of complex 2

Biography

Daniela Gutiérrez completed her Bachelor's degree at the Universidad Autónoma de Puebla (México) in 2015. She is pursuing Master's degree in Biochemistry and Molecular Biology. Her research interests are the synthesis of metallic complexes by using Green Chemistry methods and their application in the biology field.

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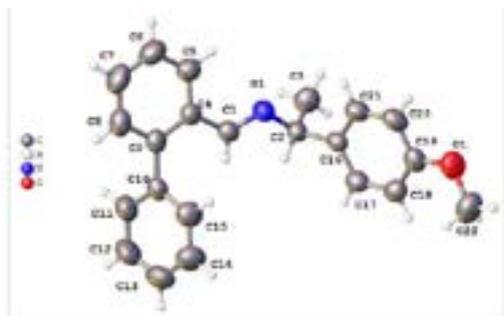
Green synthesis of a chiral imine and its Pd(II) complex

Gloria E Moreno, Guadalupe Hernández, Daniela Gutiérrez, Oscar Portillo and René Gutiérrez
Universidad Autónoma de Puebla, México

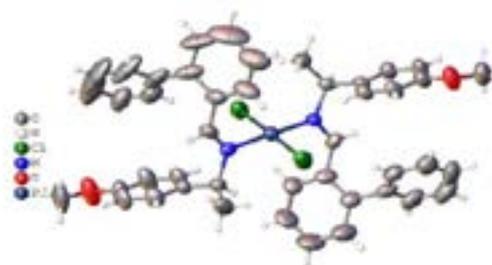
Statement of the Problem: Schiff base compounds are widely studied and used, attracting much attention in both organic synthesis and metal ion complexation. Recently we have focused our attention on the synthesis of chiral Schiff bases by using green techniques.

Methodology: We synthesized a new chiral imine using the solvent-free approach. The reaction occurs under mild conditions and requires easier workup procedures and simpler equipment, compared to similar reactions carried-out in solution. On the other hand, the ever increasing interest in Pd(II) complexes stems from their useful applications in many areas such as materials science, determination of enantiomeric excesses and absolute configuration of chiral compounds, asymmetric synthesis, etc.

Findings: The reaction of the enantiopure imine ligand leads to the formation of a new palladium complex, and both the compounds have been characterized by IR, ¹H and ¹³C NMR, MS-FAB+. The crystal and molecular structure for the palladium complex derived from imine obtained with biphenyl-2-carboxaldehyde and S-(-)-4-methoxymethylbencylamine, has been confirmed by X-ray analysis. Further discussion on these complexes will be provided.



Crystal structure of the imine



Crystal structure of the Pd (II) complex

Biography

Gloria E Moreno obtained her PhD in Chemical Sciences at the Universidad Autónoma de Puebla. She has experience in research and teaching at the Faculty of Chemistry Engineering and she is one of the members of the Laboratorio de Síntesis de Complejos. Her research interests include the synthesis and characterization of organometallic compounds by using Green Chemistry methods.

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Notes:

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Solvent-free mechanochemical obtention of phenol-N-aminal aggregates

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Phenols and cyclic aminals are known to form a variety of supramolecular aggregates via O—H...N hydrogen bonds, and complexes of phenols with various nitrogen bases are model systems often applied in the study of the nature of the hydrogen bond. Previously, hydrogen bonding between the hydroxyl group of acidic groups such as phenols and heterocyclic nitrogen atoms has proved to be a useful and powerful organizing force for the formation of supramolecules. The phenol–N complex has also served as a good model for the investigation of proton and electron-transfer processes occurring in living matter, it being generally assumed that this interaction consists solely of the attraction between the lone pair of the amine N atom and the phenolic hydroxy proton. In addition to the typical features of intermolecular hydrogen bonding, these systems have an extra advantage over many other complexes because they play an important role in probing the anomeric effect in N—C—N (aminal) systems even though the anomeric effect is well recognized as an important factor in defining the predominant conformational state of many cyclic heteroatom containing compounds. Noteworthy, usually cyclic aminals react with phenols when the reaction is attempted under standard conditions in various organic solvents affording symmetrical imidazolidines in good yields. We discovered that, under mechanochemical conditions, grinding the reagents in a mortar and pestle, the reaction of some cage type aminals with phenols affords phenol–aminal aggregates in excellent yields. Furthermore, no side products form in the reaction mixture. Usually, washing the homogeneous mixture with an appropriate solvent and filtration of the solid gives the pure adduct. This mechanochemical process provides a convenient and efficient method to produce these adducts, and is also environmentally friendly.

Biography

John Sadat-Bernal studied Chemistry at the Universidad Nacional de Colombia. He received his PhD degree in Chemistry from Universidad Nacional de Colombia where he worked on his thesis entitled, 'synthesis of N-containing heterocyclic compounds'. He joined the Universidad Militar Nueva Granada (UMNG) as a Professor and Researcher 3 years ago and his research interest focuses mainly on heterocyclic synthesis and analytical methods.

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Notes:

Solvent-free procedure for the synthesis of tetrahydrosalen (H4salen) ligands by a solid state reaction using sodium borohydride as a reducing agent

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N,N'-bis(2-hydroxybenzyl) and N,N'-dibenzyl derivatives of 1,2, and 1,3-diamines, also known as tetrahydrosalen or salan ligands, are intimately involved with a number of metal coordination complexes, which include those elements located in groups 12, 13 and 14. These tetradentate ligands associated with metal centers display cis-octahedral coordination geometry, which can form two possible diastereomers (*cis fac-mer* and *cis fac-fac*), forming octahedral chiral complexes of the type $[\{ONNO\}MX_2]$. Different methods have been developed for the preparation of this class of compounds but the reduction of the corresponding diimines offers the possibility to produce a wide range of such diamines. A series of N,N'-dibenzyl or N,N'-(2-hydroxybenzyl)- ethane-1,2-diamine, -propane-1,3-diamine and -1,3-diamino-2-propanol (TetrahydroSalen ligands) were prepared in good yield by an efficient and highly eco-friendly protocol. The respective di-Schiff bases (Salen) precursors were prepared in good yield by using water as a solvent without the need for catalysis or the azeotropic removal of water. The reduction with sodium borohydride of the respective di-Schiff bases under catalyst-free and solvent-free conditions occurs readily and with good yields, ranging from 48% to 95%. The direct solid-solid reductive aminations were carried out by grinding the corresponding di-Schiff base and sodium borohydride with an agate mortar and pestle at room temperature. Then, the reactions were conducted by heating at 60-90°C on a hot plate and were complete within 15 minutes, producing tetrahydro-di-Schiff bases compounds. Compared to the previously reported methodologies, our protocol offers considerable benefits, including that it has a simple procedure, is environmentally benign, produces high yields, does not require the use of a catalyst, and allows for the product to be synthesized on the gram scale.

Biography

Jaime Ríos-Motta has his expertise in synthesis of heterocyclic compounds based on the use of a minimal cage as preformed Mannich reagents. He has completed his PhD from the National University of Colombia. He belongs to the group of research in synthesis of heterocycles as Senior Investigator. He has published more than 80 papers in reputed journals and has been serving as an Editorial Board Member of reputed journals.

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Green synthetic approaches for medium ring-sized and linear benzylimidazolidine oligomers

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Aminophenol-type Mannich bases are of great chemical and industrial interest due to their growing applicability for the production of new polymeric materials with excellent mechanical, thermal, photophysical, and catalytic properties. The reaction between the phenolic Mannich bases 1,3-bis[2'-hydroxybenzyl]imidazolidines and the macrocyclic amina 1,3,6,8-tetraazatricyclo[4.4.1.13,8]dodecane (TATD) - a preformed Mannich base - was studied under solvent-free conditions. The solvent-free Mannich-type aromatic reaction between the macrocyclic amina TATD and Mannich phenolic bases of the type 1,3-bis[2'-hydroxybenzyl]imidazolidine is a useful synthetic strategy for the high-efficiency production of medium ring-sized heterocalixarene-type compounds and linear oligomers which contains at least three benzylimidazolidine units. In addition, it was possible to get access to oligomers which could not be prepared via several different standard procedures. The 1,3-bis[2'-hydroxybenzyl]imidazolidines used were prepared by a solvent-free Mannich-type condensation between the macrocyclic amina TATD and the appropriate phenol. Besides, macrocyclic amina TATD was prepared and isolated in pure water in high yield and purity. The preparation of TATD in water becomes important due to environmental consideration. This is a simple method to prepare cyclic and linear oligomers in good yield and high purity under solvent-free conditions without the presence of any organic solvent or catalyst.

Biography

Augusto Rivera received his Bachelor's in Chemistry and Doctorate degree from Universidad Nacional de Colombia in 1976 and Universidad de La Laguna at Tenerife, Spain in 1979 respectively. He returned (1980) to the Universidad Nacional de Colombia where he became Full Professor. He has over 150 publications that have been cited over 800 times, and his publication H-index is 16. His research interests are in the area of N-containing medium-ring compounds, design of novel amins, new synthetic methodologies and solid-state organic reactions.

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Prediction of cellulose dissolution in ionic liquids using molecular descriptors based QSAR model

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Statement of the Problem: The dissolution of lignocellulose by ionic liquids attracted much attention during the last decade. However, the experimental screening and selection of a large number of potential ionic liquids for biomass processing are challenging tasks.

Methodology & Theoretical Orientation: In this work, the prediction of cellulose dissolution in ionic liquids (ILs) was evaluated by quantitative structure-activity relationship (QSAR) model using the molecular descriptors of ionic liquid's constitutional ions derived from Comprehensive Descriptors for Structural and Statistical Analysis (CODESSA) program. All the structures of individual cations and anions of ILs were optimized without constraint using B3LYP/6-31G(d,p) level in Gaussian 03 package and verified as minima by frequency calculations. The CODESSA package calculates various descriptors such as constitutional, topological, geometrical, electrostatic, quantum-chemical, and thermodynamic from the three-dimensional structures of molecules. 438 molecular descriptors were calculated for 80 different ILS in the data set.

Findings: Two QSAR correlation models for cellulose solubility in ILs with respect to mass and molar percentages were developed. Both models include 13 molecular descriptors and were reliable as indicated by the considerably high R^2 value for both training and test sets. Models based on cellulose molar solubility exhibited better correlation (R^2 of 0.92 vs. 0.88) and predictability (R^2 of 0.89 vs. 0.83) than those based on mass percentage solubility.

Conclusion & Significance: These results indicated that the molecular descriptors of ILs could be effectively used to develop QSAR models for facilitating the in silico and a prior screening/selection of ILs customized for specific applications.

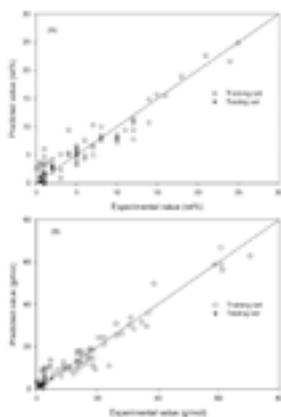


Figure: Scatter plots of predicted vs. experimental values of cellulose solubility in ionic liquids

Biography

Chan Kyung Kim is a Professor and Chairman of the Department of Chemistry, Inha University located in Incheon, Korea. He is an active member of Brain Korea 21 Plus Project supported by the Ministry of Education, Science and Technology. His research is concentrated on the development and application of QSAR/QSPR method including MSEP for high energy density materials. He is also interested in the theoretical organic and inorganic chemistries to understand the structures and reactivity of chemical systems. Recently, his research is oriented on the design of carbon dioxide removal in the presence of N-methylaniline and silyl halides and conversion of carbon dioxide to some useful materials in the zeolite catalysts.

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Methane steam reforming through shell-and-tube heat exchanging reformer to improve heat transfer rate from low temperature heat source

Sangseok Yu and Jinwon Yun

Chungnam National University, South Korea

In the renewable energy technology, methane steam reforming is used to supply hydrogen rich fuel to fuel cell system that has high temperature heat source with conventional burner. The methane steam reforming technology is also used as secondary reformer to improve system efficiency with utilization of wasted thermal energy. When the heat source temperature is low, the heat transfer mechanism is very crucial to improve reforming reaction rate. At very low temperature such as 500°C, it is known that the methane conversion rate of steam reforming reaction is severely deviated from equilibrium. In this study, the heat exchanger design is investigated to improve methane conversion rate of low temperature secondary steam reformer. Right after the numerical model is validated with experimental data, the analysis is mainly concentrated on the various heat transfer parameters so that the principle parameter could be determined. Results show that since the temperature distribution in longitudinal and radial direction is sometimes severely non-uniform under practical environmental and operating conditions, the methane conversion rate is strongly depended on the non-uniformity. Result also shows that large steam to carbon ratio of practical steam reformer sacrifices thermal duties so that methane conversion rate has trade-off over increasing steam to carbon ratio.

Biography

Sangseok Yu is a Professor of Mechanical Engineering at CNU who is an expert in modeling and simulation of energy system. He majored in transient heat and mass transfer and dynamic modeling of automotive fuel cell system at University of Michigan Ann Arbor. In particular, he has special interests in control and fault detection of automotive fuel cell system. Recently, he extended his research scope to modeling and simulation of various energy systems.

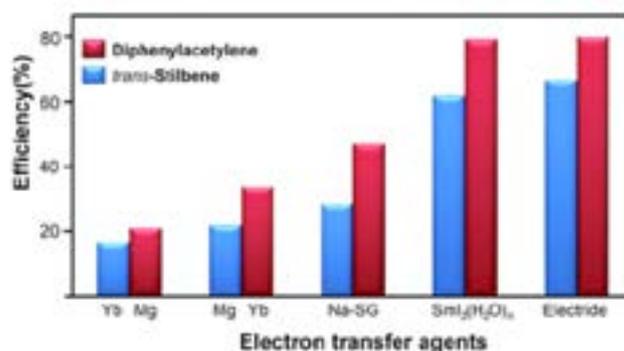
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Two-dimensional inorganic electride promoted electron transfer efficiency in transfer hydrogen reactions of carbon-carbon multiple bonds

Ye Ji Kim, Byung Il You and Sung Wng Kim
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The development of simple and efficient chemical transformation routes with maximal yields has been a continuously pursued challenge in synthetic chemistry. Such protocols can provide important benefits in the field of organic synthesis such as saving starting materials, reagents, and energy, thereby lowering production costs and environmental impacts. Among fundamental reactions in synthetic organic chemistry, the reduction of organic functional groups with carbon-carbon (C-C) multiple bonds is one of the most universally applied and crucial synthetic processes in academic and industrial circles. For efficient electron transfer hydrogenation, it is essential to use an agent with a high reduction potential to facilitate the electron transfer. In this regard, many types of materials, such as simple metals (Mg and Yb), stabilized alkali metal systems (Na in silica-gel and in ammonia liquid), and lanthanide iodides (SmI₂ and TmI₂), have been employed in electron transfer hydrogenation. Despite their effectiveness in the reported transfer hydrogenations, there are several drawbacks in the methodology. Major disadvantages include the toxicity, the cost of agents and the rigorous reaction conditions. Furthermore, the separation of products from the resultants is laborious and inefficient, yielding pollutants. Of all these drawbacks, the low electron transfer efficiency of the reaction is the most critical issue to be addressed for efficient transfer hydrogenation. In this presentation, we will introduce simple and highly efficient transfer hydrogenation of alkynes and alkenes by using a two-dimensional electride, dicalcium nitride ([Ca₂N]^{+•e-}), as an electron transfer agent. Excellent yields in the transformation are attributed to the remarkable electron transfer efficiency in the electride-mediated reactions. We found that the choice of solvent was crucial for enhancing the electron transfer efficiency, and a maximum efficiency of 80% was achieved by using a DMF mixed isopropanol co-solvent system. This is the highest value reported to date among single electron transfer agents in the reduction of C-C multiple bonds.



Biography

Ye Ji Kim got her Bachelor's degree in Chemistry from Kyungsoo University in 2013. Since 2013, she joined prof. Sung Wng Kim's group of Sungkyunkwan University as Post-Graduate student. Her research interest includes chemical application of inorganic electride, single electron transfer reaction, hydrogen evolution reaction and nano-particle fabrication.

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Enhanced GABA production via protein complex of *Pyrococcus horikoshii* glutamate decarboxylase and *Escherichia coli* GABA transporter

Soon Ho Hong

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Gamma-aminobutyric acid (GABA) is a precursor to pyrrolidone, a monomer used for the production of a biodegradable polymer known as nylon-4. GABA is also widely used in the medical industry to treat conditions such as high blood pressure, anxiety and depression. Generally, GABA is produced from glutamate by the enzyme glutamate decarboxylase (GadB). In this study, a synthetic scaffold complex was introduced between *Pyrococcus horikoshii* GadB and the GABA antiporter (GadC) from *E. coli*. *P. horikoshii* GadB was attached to the N-terminus, C-terminus and middle of *E. coli* GadC via scaffolding. Among the three scaffold complexes evaluated, the N-terminus scaffold model produced 5.93 g/L of GABA from 10 g/L monosodium glutamate (MSG). When the gabT mutant *E. coli* XBT strain was used, the highest GABA concentration of 5.96 g/L was obtained, which is 97.8% of GABA yield. In addition to GABA concentration, GABA productivity was increased 3.5 fold via the synthetic scaffold complex.

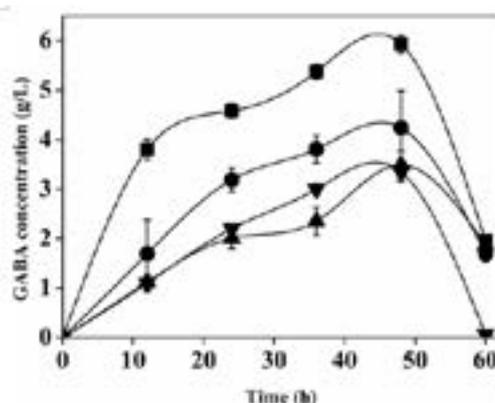


Fig. 1. Time profile of GABA production for 60 h of culture from various scaffold complexes, pH1BP : N-terminus scaffold complex (■), pH2BP : Sandwich scaffold complex (●), pH3BP : C-terminus scaffold complex (▲), pHBP : Without scaffold complex (▼).

Biography

Soong Ho Hong graduated from School of Chemical Engineering & Bioengineering, University of Ulsan, Korea. His major research field involves Metabolic Engineering, In Silico Simulation of Microorganisms, Systems Biology, Synthetic Biology, and Bioengineering.

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Notes:

Ammonia borane as hydrogen storage material: Study of some of its clusters

Cacier Zilahy Hadad, Andy Zapata and Albeiro Restrepo
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Hydrogen is one of the most promising alternatives as clean fuel. This is because the energy, per unit of fuel mass, released in its reaction with oxygen is higher than that of gasoline, and the chemical product of this combustion is only water. Nevertheless, hydrogen storage methods are still inefficient and expensive. Ammonia borane (AB = H₃N-BH₃) has emerged as one of the most encouraging hydrogen storage materials due to its relative stability, its versatility, and its capacity of storing high hydrogen densities. However, a series of scientific and technological problems that prevent its use for this purpose remain to be solved. To name one, the methods known today for extracting hydrogen from AB are still insufficient: there is not yet one in which a total hydrogen release from AB is guaranteed at relatively low temperatures. To better address these and others current problems, it would be crucial to know, very precisely, what the structural nature and the intra- and intermolecular interactions involved in AB are. In this work, from a quantum-mechanics point of view, we contribute to this task, revealing important aspects not found by previous studies. A search for stable configurations was performed on the trimers, (AB)₃, tetramers, (AB)₄ and pentamers, (AB)₅, of ammonia borane at high levels of theory. Very rich and complex potential energy surfaces, PESs, are obtained. Cyclic or compact configurations are energetically preferred. Four different types of non-conventional interactions are identified: heteropolar N-H \cdots H-B dihydrogen bonds (the main stabilizing factor), homopolar B-H \cdots H-B dihydrogen bonds, and B \cdots H-N and N \cdots HB hydrogen bonds. Donor-acceptor charge transfer in heteropolar dihydrogen bonds is the most stabilizing interaction, taking place between a σ – bonding orbital and a σ^* – anti-bonding one. Despite H \cdots H being a priori considered as weak interaction, stabilization energies in ammonia borane clusters are comparable to the interactions responsible for the stabilization of water clusters at the same level to theory.

Biography

Cacier Z Hadad has completed his PhD at the University of Chile. He is the Co-Head of the Theoretical Chemical Physics Group of the University of Antioquia, Colombia. He is author of many relevant papers about theoretical aspects and models of diverse physicochemical phenomena.

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Notes:

Accelerated solvent extraction as an alternative tool for extraction of chlorogenic acid from *Cynara scolymus* leaves

Ibrahim Ahmed Saleh¹, Nahla Sayed Abdel-Azim¹, Khaled Ahmed Shams¹, Elsayed Aboutabl², Faiza Mohamed Hammouda¹, Mohamed-Elamir Fathy Hegazy¹ and Tarik Abdelhalim Mohamed¹

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Finding new techniques to enhance the extraction efficiency of bioactive compounds from medicinal and aromatic plants (MAPs) is important due to their potential health benefits. The objective of this study was to evaluate extractability of chlorogenic acid from *Cynara scolymus* leaves using solvents under high pressure and temperature. Accelerated Solvent Extraction (ASE) is considered as a greener method for MAPs extraction when compared to conventional extraction technique. ASE is an extraction technique which combines both elevated pressure and temperature. Methodology & Theoretical Orientation: Chlorogenic acid from *Cynara scolymus* leaves was extracted using ASE applying one and three static cycles of extraction at 40, 80, and 120 °C. Static periods of extraction were carried out for 5, 10 and 15 min using 80% methanol/water (v/v) as the extraction solvent. The extracted solutions were characterized for chlorogenic acid content by HPLC. Findings: The highest chlorogenic acid yields were obtained after 10 min (67.4 and 66.8 mg/5g DM) using one and three static cycles of extraction; respectively. Accelerated Solvent Extraction (ASE) has proven to be an effective extraction technique. However its recommended not to exceed the extraction time over 10 min at elevated temperatures, due to the possible degradation of chlorogenic acid for prolonged extraction at extreme conditions.

Biography

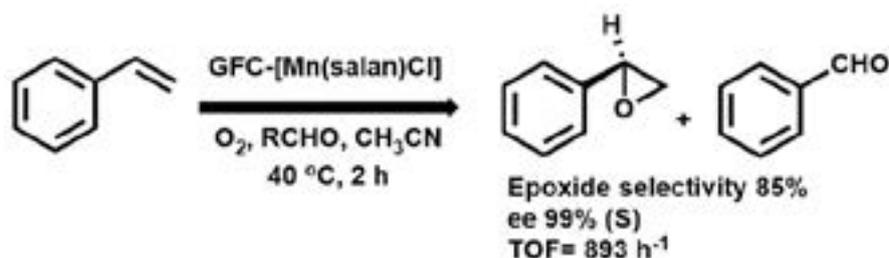
Ibrahim Saleh, Researcher, Phytochemistry Department, National Research Centre, Egypt, has awarded his Ph.D degree from faculty of pharmacy, Cairo University, Egypt. He has awarded international scholarship as an academic visitor, Coventry University, Coventry, United Kingdom. During the last ten years, he has been publishing in the area of natural products chemistry, his program has come to focus on innovation and development of medicinal and aromatic plant processing.

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Manganese-salan complex immobilized on reduced graphene oxide: A recyclable catalyst for aerobic enantioselective epoxidation of olefinsHassan Hosseini-Monfared and Vahideh Abbasi
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Chiral compounds are commonly required in pharma, agrochemical and fine chemical sectors. More importantly, there is a strong demand for the pure enantiomers in pharmaceutical industry. Various desirable chiral products can be synthesized using chiral epoxides by stereospecific ring-opening reactions. Catalytic asymmetric oxidation of olefins by various oxygen donors can be used to prepare chiral epoxides. From the point of view of green and sustainable chemistry, molecular oxygen is an ideal oxidant with regard to its natural, inexpensive and environmentally friendly characters. Salen (bis(salicylidene)ethylenediamine) and salan (N,N'-bis(o-hydroxybenzyl)-1,2-diaminocyclohexane) ligands are an important class of tetradentate dianionic ligands in the chemistry of transition metals. Chiral salans have been known as effective ligands for asymmetric synthesis because of their more flexibility which let to be modified easily with respect to salen ligands. Chiral salan compounds have been used as a fluorescent sensor for CuCl and salan-Cu complex for the selective recognition and discrimination of protected α -amino acids. In this study, a chiral Mn(III) complex of the reduced salen ligand (salen = (1R,2R)-(-)-(N,N'-bis(5-chloromethylsalicylidene)cyclohexane-diamine) was synthesized and covalently grafted onto carbon coated magnetic Fe₃O₄ nanoparticles decorated reduced graphene oxide sheets (GFC). The catalyst was characterized by FT-IR, UV/Vis, XRD, SEM and vibrating sample magnetometer (VSM) techniques. The synthesized GFC-[Mn(salan)Cl] was employed in the aerobic enantioselective epoxidation of non-functionalized olefins. The effects of reaction variables such as temperature, time and solvent on the catalytic performance were systematically investigated. The catalyst was found to be highly active and enantioselective for epoxidation of styrene (Scheme 1), alpha-methyl styrene and trans-stilbene. Catalyst GFC-[Mn(salan)Cl] is stable and could be recycled at least five times without loss of its catalytic activity.

Scheme 1: Catalytic oxidation of styrene with O₂.**Biography**

Hassan Hosseini-Monfared has research focus on applied homogeneous and nanostructured heterogeneous catalysis, the development and application of new, environmentally benign catalysts, asymmetric catalysis and synthetic methods.

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Notes:

Comparison of net GHG emissions between separated system and crop-swine integrated system in the North China plain

Zhejin Li

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Agriculture causes 10–12% of global GHG (CO₂, CH₄ and N₂O) emissions. GHG emissions from Chinese agriculture have been estimated at 819.97 Mt CO₂-equivalence (CO₂-eq); among them, total annual GHG emissions from the production of grain and livestock have been estimated at 374 Mt CO₂-eq and 445 Mt CO₂-eq, respectively. Because of food demand, food production has intensified, resulting in the separation of crop production and livestock rearing. This separation has increased the application of outside resources and agricultural waste, aggravating GHG emissions and other ecological and environmental problems. This research attempts to mitigate GHG emissions by improving soil carbon sequestration of crop production and decreasing emissions from swine-rearing waste. Net GHG emissions (NGHGE) between an integrated system and a separated system are compared in this study from a life-cycle perspective. The causes of different GHG emissions between these two systems are analyzed and mitigation strategies are proposed. The results show that the NGHGE of crop-swine integrated and separated systems were 24917.95 kg CO₂-eq/ha/yr and 27732.70 kg CO₂-eq/ha/yr, respectively, for 215 head of pigs. The integrated system reduced GHG by 1381.33 kg CO₂-eq/yr mainly due to the recycling and reuse of pig manure in croplands. Meanwhile, the integrated system increased soil carbon storage by 35.92% compared with the separated system, although it increased soil CH₄ and N₂O emissions. In conclusion, these results indicate that through a series of methods, such as recycling agricultural waste, the integrated system can reduce net GHG emissions by 10.15% compared with separated systems. Although much work remains to adopt the integrated system to reduce GHG emissions, the crop-swine integrated system should be given priority to mitigate anthropogenic net GHG emissions.

Biography

Zhejin Li is a student of China Agricultural University pursuing Doctoral degree. Her major is Agricultural Wastes Managements and Ecological Agriculture.

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Notes:

Dehydration of sugars from grape juice waste by microwave radiationAlmudena Lorente, Covadonga Lucas-Torres and Maria Prado Sanchez-Verdu
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In Spain, grape industry is the widest, and therefore, the one that generates the larger amount of by-products. The composition depends on the grape variety used, although that is mainly water (70-80%), and sugars (20%), specifically glucose, fructose and sucrose, being the rest organic acids such as tartaric, malic or citric. The main reasons for converting those residues are their low pH and their high BDO (80-89 g/L for white juice, 78-99 g/L for red juice) and high QDO (115-117 g/L for both varieties). We propose the development of a methodology for the dehydration of the sugars in the grape juice waste water, to obtain 5-hydroxymethylfurfural (HMF) and levulinic acid (LA) as main products. Those chemicals have a great interest as platform compounds, with several applications in the biofuel industry among others. Preliminary studies were carried out on the pure monosaccharides (glucose and fructose). The solution (known concentration) was introduced in a microwave vessel and sealed with a cap for under pressure work. The required heterogeneous catalyst was added (see table 1) and the reaction set at 200°C for 2-15 minutes depending on the sugar. The reaction crude was dissolved in D₂O to be analysed and quantified by NMR. The same experiments were carried out, under the optimal conditions, on several non-edible grape juices, which were provided as a similar residue to waste water sidestreams. The preliminary studies with fructose and glucose showed that the montmorillonites as catalysts offer the best results. The reactions carried out with grape juice using montmorillonite KSF were successful in obtaining HMF and LA with a fast dehydration of fructose and a moderate dehydration of glucose. Also, the catalyst is potentially recyclable which was assessed by several experiments, showing also a moderate conversion. In this work, we have been able to obtain HMF and LA as biofuel precursors using an alternative energy source and a potentially recyclable catalyst. Although it shows less efficiency on reusing, it is clean and cheap, and allows us to simply separate it from the reaction media.

Table 1: Results for the microwave conversion of 2M fructose

Exp	Catalyst	Conversion (%)	Yield HMF (%)	Yield LA (%)	Select. HMF (%)	Select. LA (%)
1	MK10	72.2	9.7	2.7	78.2	21.8
2	M-KSF	73.8	9.4	5.9	61.5	38.5
3	Amberlyst 15	27.7	1.6	0.2	90.0	10.0
4	AmB15 10 mltr	49.8	7.1	1.5	82.2	17.8
5	Bentonite	56.4	2.9	0	100	0
6	-	35.6	0.9	0	100	0

Biography

Almudena Lorente obtained her degree in Chemistry (June 2014) at the University of Castilla La Mancha. Her first contact with Organic Chemistry was in her fifth year of degree in the group of Organic Green Chemistry and Food and Agro-Industrial Waste Chemistry. Then in November 2014, she started her PhD in the same group. During these years, she has continued her training in the field of Waste and Bioeconomy. She obtained her certificate in Bioeconomy studies in September 2016.

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Notes:

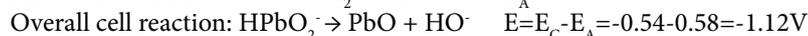
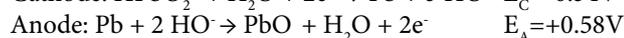
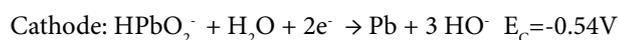
Structure and electrochemical properties of recycled active electrodes from spent lead acid battery and modified with different manganese dioxide contents

Simona Rada^{1,2}, C Denisa¹, H Vermesan¹, M Rada², P Pascuta¹ and E Culea¹

¹Technical University of Cluj-Napoca, Romania

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Manganese (IV) oxide was widely studied due to their technological importance for catalytic and electrochemical applications. The addition of MnO₂ to the active electrodes structure of the disassembled car battery is expected to give new possibilities to extend the properties of these materials by modifying their structure. The structural role of manganese ions in many oxide glasses is unique. These ions exist in different valence states with different coordination numbers simultaneously in the host network, which is mainly responsible for significant changes in the structure and physical properties. MnO₂ incorporated into active electrodes structure of the disassembled car batteries were prepared by classical melt-quenching method. The effect of MnO₂ concentration on the obtained samples was investigated by X-ray diffraction (XRD) analysis, Fourier Transform InfraRed (FTIR) spectroscopy and measurements of Cyclic Voltammetry (CV). The analysis of IR data shows that at lower MnO₂ contents, MnO₂ breaks Pb-O-Pb bonds and produces to the formation of non-bridging oxygen atoms together with the defects known as dangling bonds. At higher MnO₂ content, MnO₂ plays a network former role, joins the vitreous network as [MnO₄] and [MnO₆] structural units. The main reactions for the cathode and anode respectively can be expressed as:



In this case, the potential difference, E between cathodic and anodic reaction is -1.12V.

Biography

Simona Rada is currently working as a Professor in the Department of Physics and Chemistry, Faculty of Material Engineering and Environment, Technical University of Cluj-Napoca, Romania. She completed her PhD in Chemistry with Inorganic Chemistry specialization. She has been part of many international conferences and published many scientific papers in many reputed journals.

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Notes:

Survey analysis of dental ceramic materials based on yttria oxide-stabilized zirconia

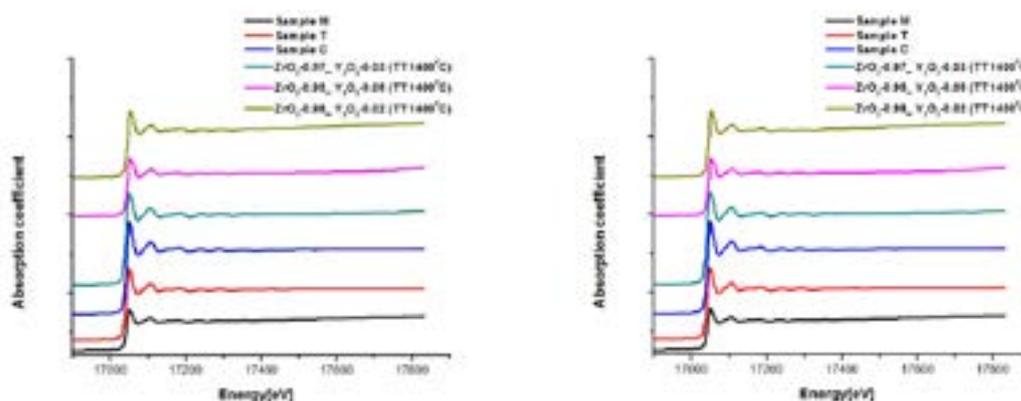
Marius Rada¹, Wu Zhonghua³, Jing Zhang³, A Bot¹, M Zagrai¹ and S Rada^{1,2}

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Statement of the Problem: The special properties of ceramic materials are becoming increasingly important for many applications in electrical, chemical and mechanical engineering. Oxide ceramic materials are used in a wide range of industries, including mining, aerospace, electronics, medicine, etc. These materials show a high strength and hardness, as well as a thermal, cracking, and corrosion resistance. Ceramics are considered as popular engineering materials due to their excellent mechanical properties: good fracture toughness, high strength, elastic modulus, and wear resistance, used in many engineering applications such as engine elements, valves, cutting tools, and moulds. In recent years, YSZ with its superior combination of mechanical properties and chemical inertness has been employed in the biomedical field as an implant material. The main aim of the present study is to investigate how the yttrium (III) oxide can influence the formation of monoclinic zirconia crystalline phase in ceramics. The ceramic systems in the xY_2O_3 (100-x)ZrO₂ compositions where x= 2,3 and 5% Y₂O₃ were synthesized by sintering method in alumina crucibles at 1400°C for two hours. For this work, we compared the samples obtained in our laboratory with those used in the medical market, called sample M, T and C. For all samples were characterized by investigations of XRD, and XAS analysis. The EXAFS analysis of absorption coefficient was processed by computer codes CDXAS, XAS and IFEFFIT.



Biography

Marius Rada is Senior Research Scientist II at The National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania. As a Scientist Researcher or Principal Investigator, he led a number of national research grants, in the areas of material science with applications in the recycling of the car batteries and dental ceramics. He has published over 45 papers in ISI journals and has published 1 book and 2 chapters of the book.

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Low-temperature hydrogenation of carbon dioxide to methanol using a homogeneous cobalt catalyst

Rauf Razaq

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Methanol attracts significant attention as a hydrogen storage material (12.5 wt % H₂), drop-in liquid fuel as well as an energy carrier in methanol fuel cells. Its industrial utility combined with these promising energy applications has led to multiple proposals of a so-called “Methanol Economy” in which methanol would be the central carbon and energy feedstock in a sustainable energy economy. Currently, methanol is produced from fossil fuels, especially natural gas, via syngas (mixture of CO, CO₂ and H₂). For a more sustainable production of methanol direct reduction of CO₂ is a highly interesting option if green hydrogen or renewable energy is used. In such a way it would be possible to recycle atmospheric carbon as part of a carbon capture and recycling strategy (CCR), avoiding additional CO₂ emissions and replacing non-sustainable carbon sources. So far, hydrogenation of CO₂ to methanol has been studied intensively using heterogeneous catalysts. Hence, a large library of active catalysts has been developed but most require high temperatures (>200 °C) to operate. Herein, we describe the first homogeneous non-noble metal catalyst for the hydrogenation of CO₂ to methanol. The *in-situ* formed catalyst based on Co(acac)₃/Triphos/HNTf₂ allows to perform the reaction at 100 °C without a decrease in activity. Kinetic, *in-situ* NMR and MS studies suggest an inner-sphere mechanism catalyzed by a cationic cobalt/Triphos complex, which is formed after slow removal of the acac ligands. We hope that this report will inspire the development of novel, homogeneous non-noble metal based catalysts for a cost and energy efficient hydrogenation of CO₂ to methanol.

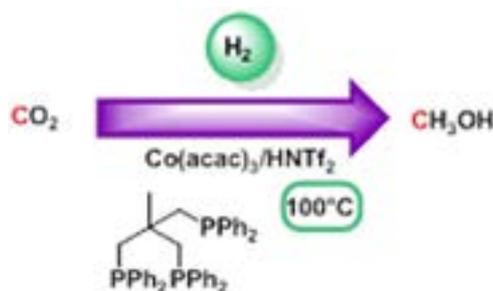


Figure: Low-Temperature Hydrogenation of Carbon dioxide to Methanol Using a Homogeneous Cobalt Catalyst

Biography

Rauf Razaq has his expertise in both Homogeneous and Heterogeneous Catalysis: material design, synthesis and application. Recently, Mr. Razaq is busy with designing novel catalytic systems for efficient CO₂ valorization. He has also good experience in chemical reaction engineering and reactor design. During his research he has not only studied the effect of various metals in catalyzing the CO₂ hydrogenation reaction but has done some extensive work on understanding the influence of the type of catalytic reactor during such reactions. This approach carries a significant importance in applied catalysis especially in scale-up from lab to pilot and then industrial scale.

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Notes:

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Liting Yang et al., Trends in Green chem, 3:2
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Metal-free aerobic oxidative coupling of thiols for synthesis of disulfides and sulfenamides

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

Statement of the Problem: Catalytic synthesis of organic sulfenamides and disulfides has great significance and value in synthetic chemistry and bioscience. Despite the prominent applications of sulfenamides, there are only a few reports about their preparation. In this contribution, we reported an oxidative coupling of 2-mercaptobenzothiazole leading to 2,2-disbenzothiazoledisulfide in up to 94 % yield.

Findings: The reactions used TEMPO as the catalyst and underwent a radical mediated process. Inspired by that finding, we explored the radical reaction between thiols and amines. Fortunately, we found a TEMPO-catalyzed aerobic oxidative coupling system, which utilizes environmentally friendly and naturally abundant O₂, producing sulfenamides and disulfides in high yields. Reactions showed good tolerance toward various amines and thiols. Activation of the N-H bond by 2,2-disbenzothiazoledisulfide showed the great potential in organic synthesis.

Conclusion & Significance: We successfully developed a highly efficient and sustainable metal-free radical-mediated method to generate compounds containing S-N and S-S bonds in high yields. The TEMPO-catalyzed aerobic oxidative homocoupling of thiols or heterocoupling of thiols with amines provides a new prospect for large-scale syntheses of disulfides and sulfenamides, such as rubber accelerator TBBS, which is required in metric tons worldwide each year.

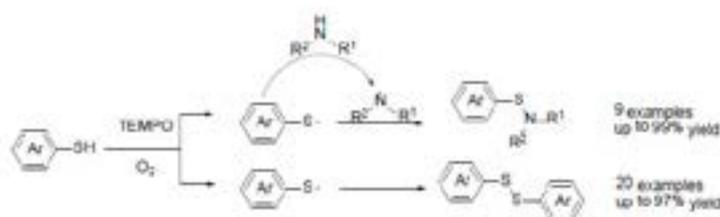


Figure 1. TEMPO-catalyzed coupling of thiols for metal-free formation of S-N/S-S bonds under the oxidation of oxygen

Biography

Liting Yang is pursuing her PHD at College of Chemistry and Molecular Engineering, Zhengzhou University, China. She obtained Bachelor's degree of Chemistry at 2011 from Zhengzhou University. Starting from 2011 to present, she has been working on scientific research in the group of Professor Guanyu Yang. The main research fields contain the synthesis and application of radical catalysis and aerobic oxidative green-catalyzed construction of S-N/S-S bonds. Some of the research achievements have been published on the international journals, such as Green Chemistry, Asian Journal of Organic Chemistry and so on.

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Biography

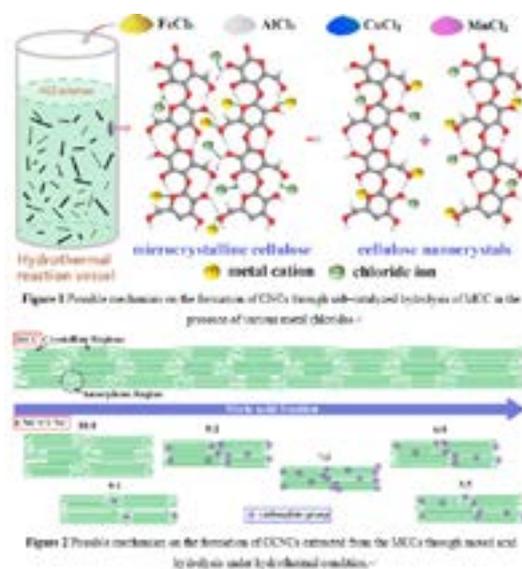
Guanyu Yang is a Professor in College of Chemistry and Molecular Engineering, Zhengzhou University, China, since 2006. He received his Ph.D. of chemistry in 2005 from Dalian Institute of Physical Chemistry, Chinese Academy of Sciences. His research interests center around the development of new synthetic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

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Efficient extraction and functionalization of cellulose nanocrystals through hydrochloric acid hydrolysis under hydrothermal conditions

Miao Cheng and Zongyi Qin
 Donghua University, China

A facile and efficient approach to prepare cellulose nanocrystals (CNCs) is presented through hydrothermal procedure by using inorganic chlorides as catalyst. The role of inorganic chlorides including ferric chloride hexahydrate ($\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$), copper chloride dihydrate ($\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$), aluminum chloride (AlCl_3) and manganese chloride tetrahydrate ($\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$) played on the extraction and properties of high quality CNCs were determined. It is observed that the introduction of inorganic chlorides obviously enhanced the hydrolysis process through faster degradation of disordered region of cellulose. Compared with those for pure hydrochloric acid hydrolysis, smaller diameter and larger length to diameter ratio of CNCs could be obtained through salt-catalyzed hydrolysis. In addition, carboxylated cellulose nanocrystals (CCNCs) could be obtained by a similar one-step procedure through a mixed acid system of hydrochloric acid and nitric acid (HCl/HNO_3). It is found that the addition of nitric acid could not only promote the conversion of surface groups on the CNCs, but also have significant influences on the yield, particle size and microstructure of CNCs. For the volume ratio of HCl/HNO_3 of 7:3, the as-prepared CCNCs exhibited the largest length to diameter ratio and narrowest dimension distributions as well as maximum degree of oxidation of 0.12. Furthermore, high dispersion stability for the CCNCs could be observed due to the existence of negative carboxyl groups. These results show that the using of salt-catalyzed hydrolysis especially ferric chloride has a significant improvement on achieving high quality CNCs and the mixed acid system treatment could greatly simplify the preparation of CCNCs with high yield and high crystallinity under mild hydrothermal conditions.



Biography

Miao Cheng is a student at College of Materials Science and Engineering at Donghua University. His research interests involve the sustainable production of materials from biomass, development of high performance nanocomposites with the incorporation of cellulose nanocrystals, extraction and functionalization of cellulose nanocrystals, and all-cellulose nanocomposites.

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Assessing the vulnerability of freshwater fish in Canada's eastern boreal to climate change

Michael van Zyll de Jong and Hope Olusayna
Memorial University, Canada

Freshwater fishes are vulnerable to climate change. Due to a lack of quantitative data on status and current, and project trends for most fish species, a systematic assessment approach that incorporates expert knowledge was developed to determine status and future vulnerability of freshwater fishes to climate change in Newfoundland and Labrador, Canada. The methodological approach uses expert knowledge, supported by literature reviews of status and biology of the fishes, to score ten metrics for both (1) current status of each species (baseline vulnerability to extinction) and (2) likely future impacts of climate change (vulnerability to extinction). Baseline and climate change vulnerability scores were derived for 5 native and 2 alien species of Salmonid fishes.

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Notes:

Hydrophobic sorption of the soil treated with *giant Miscanthus*-derived biochar as a function of aging period

Seunghun Hyun, Chanyang Kim and Juhee Kim
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Biochar produced from at three different pyrolysis temperatures (400°C, 500°C and 700°C) of giant miscanthus was treated in the ratio of 5% (w/w) in soil (namely, GMC-400, GMC-500, and GMC-700, respectively) and their sorption (kinetics and isotherm) with two hydrophobic model solutes (phenanthrene (PHE) and 9-phenanthrol (9-PTR)) was evaluated as a function of aging periods (0, 3, and 6 months). Physicochemical properties of samples were assessed through the analyses of elemental composition, FT-IR, and SEM. The magnitude of PHE sorption (K_d) by samples was in the order of GMC-500 ≥ GMC-400 >> GMC-700. Sorption kinetics of PHE was apparently biphasic and GMC-500 had the largest slow sorption domain. Field aging resulted in the decreased PHE sorption (K_d) over time. Sorption of 9-PTR also decreased over time whereas its hydrophilic sorption increased from 20% up to 30% with aging period. Analyses of FTIR and SEM show that the number of O-containing functional groups increased and the deformation (or blockage) of micropores occurred after 6 months. The aging effect was most apparent for GMC-500. The result of this study strongly supports that giant miscanthus–biochar produced at 500°C is efficient adsorbent for both PHE and 9-PTR, due to its large hydrophobic surface and microporous structure. However, the sample surface became less hydrophobic due to the formation of hydrophilic functional group and the deformation of microporous structure over time due to weathering processes.

Biography

Seunghun Hyun is a Professor in the Department of Environmental Science and Ecological Engineering at Korea University since 2006. He received PhD degree from Purdue University in 2003, and received both BS and MS degrees from Korea University. His expertise is contaminant fate/clean-up in contaminated sites such as abandoned mines, landfills, spilled sites, etc. His recent research project funded by Korean Government is "Assessing long-term fate of heavy metal by understanding non-equilibrium characteristics of natural attenuation process".

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July 24-26, 2017 Rome, Italy

Characteristics of bio-oil produced by the pyrolysis of mixed waste tire and biomass

Özlem Onay

Anadolu University, Turkey

In this work, waste tire was co-pyrolyzed with biomass to investigate the effects of the waste tire on yield and chemical compositions of bio-oil product. Biomass was mixed with waste tire in the mass ratios of 0:1, 1:10, 1:4, 1:1, 4:1, 10:1 and 1:0. The pyrolysis experiment was carried out by using a lab-scale pyrolysis reactor. The experimental results showed that the addition of the waste tire led to an increase of bio-oil yield. The maximum of bio-oil yield was obtained at the waste tire/biomass mass ratio of 1:10. The characteristics of the obtained oils were studied by elemental analyzer, FTIR and GC-MS. It was found that the bio-oil obtained from the pyrolysis of mixed biomass and waste tire had higher carbon and hydrogen content, lower oxygen content than those produced by the pyrolysis of biomass alone. Moreover, there were more aromatics and aliphatic compounds in the obtained bio-oil product. These variations indicated that the existence of the waste tire significantly influenced the chemical compositions of bio-product. These variations indicated that the existence of the waste tire significantly influenced the chemical compositions of bio-oil.

Biography

Özlem Onay obtained her PhD degree in Chemical Engineering from the University of Anadolu in 2001. In 2010, she became an Associate Professor at the University of Anadolu. Currently, she is a Professor and her skills are mainly dedicated to thermal conversion processes. She also has 26 publications in international recognized journals, and 25 presentations in international conferences. Her expertise in reviewing scientific papers led her to become the Editorial Board Member of *International Journal of Petroleum Technology* and *MAYFEB Journal of Energy*.

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Notes:

Treatment of hazardous waste incineration plant effluent by novel hydrogels

Omer F Kemik¹ and Ufuk Yildiz²

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Hazardous waste disposal is one of the biggest environmental issues of last decades. Incineration is a way to disposal of hazardous wastes and has many advantages beside disadvantages. One of the most important disadvantages is effluents which contain heavy metal ions as pollutants. Unlike some other organic pollutants, heavy metals are nonbiodegradable, highly toxic and carcinogenic. In addition, due to their high solubility in water, even very low concentration results in ecological problems, so it is necessary to remove these ions. Different methods or materials have been used, new techniques and materials have been tried to develop or improve to find more effective ways to remove such ions from wastewater. Hydrogels are crosslinked hydrophilic polymers that are widely used in the purification of wastewater. Due to their high swelling in water, ability to control the diffusion process, swelling response to changes in ionic strength, pH and temperature and also the capability to bind heavy metal ions through the polar functional groups which interact selectively and strongly with heavy metal ions, moreover easy handling and reusability make hydrogels promising materials for water purification. Macroinimer which has the properties of macromonomers, macrocrosslinkers and macroinitiator in a macrostructure, was used to prepare novel hydrogels with higher metal binding capacity than present hydrogels. Novel hydrogels were prepared by oil-in-water high internal phase emulsion copolymerization of 2-hydroxy ethylmethacrylate, N-isopropylacrylamide and N,N'-methylenebis(acrylamide) as crosslinker at room temperature. Macroinimer was used as co-surfactant and co-crosslinker. Varying amounts of N-isopropylacrylamide and macroinimer were used to prepare hydrogels. Swelling properties of all hydrogels was investigated at different temperatures. Also hydrogels were used as binding materials for different heavy metals such as Pb, Cr and Hg from hazardous waste incineration plant effluent to identify the best fitting hydrogel composition for heavy metal ion binding capability.

Biography

Ömer F Kemik is a Chemist from Kocaeli, Turkey. He graduated from Kocaeli University with MSc degree in Chemistry in 2009. He is currently PhD student at Kocaeli University and also works for İZAYDAŞ which is the only hazardous waste incineration plant of Turkey. He has expertise especially in hydrogels for environmental purposes and proficiency testing in wide scope.

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Notes:

Lithium tetrathiafulvalene carboxylate assisted inductively coupled plasma mass spectrometry determination of total mercury in air particulate matter supported by electrochemical study of preservation effects

Maja Budanovic

Nanyang Technology University, Singapore

The multi-elemental analysis of mercury via inductively coupled plasma-mass spectrometry (ICP-MS) in airborne particulate matter (PM_{2.5}) is still challenging due to the lack of accuracy for the low level mercury concentrations as a result of mercury instability. Therefore, this study investigated the effect of old and new preservation agents such as gold, methionine and lithium tetrathiafulvalene carboxylate (LiCTTF) to improve the determination of mercury for trace analysis of PM_{2.5} samples. Statistical analysis revealed that a concentration of 10 µg mL⁻¹ of LiCTTF was sufficient to obtain highly accurate results with t values of 0.1044 to 1.1239 and apparent recovery of 85% to 100%. An evaluation of the method revealed mercury spiked recovery of 91% and a detection limit of 0.0562 ng mL⁻¹. The method was tested for determination of trace metals in PM_{2.5}, demonstrating rather low element concentrations for the stated location. The stated outcomes were examined by conducting electrochemical studies of *in situ* interactions of mercury with LiCTTF and Tetrathiafulvalene (TTF). Cyclic voltammetry and square-wave voltammetry analyses of mercury, and mercury in presence of LiCTTF and TTF revealed complexation between the metal and sulphur-containing compounds.

Biography

Maja Budanovic is a Post-graduate Researcher at Nanyang Technological University in Singapore and has been serving as an SINGA (Singapore International Graduate Award) Ambassador for A*STAR Agency for Science, Technology and Research. She has completed her Master's degree in Analytical and Physical Chemistry and Bachelor's degree in Chemistry from the University of Zagreb.

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Notes:

Biological nutrient removal: The effect of organic load

Tea Širac¹, Ana Mikulin¹, Ana Špehar² and Tibela Landeka Dragičević¹

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Biological Nutrient Removal (BNR) of nitrogen and phosphorus has been widely used in wastewater treatment practice to control eutrophication in receiving water bodies. The most widely used nitrogen removal methods are biological nitrification (aerobic transformation of $\text{NH}_4\text{-N}$ to $\text{NO}_2\text{-N}$ and $\text{NO}_3\text{-N}$), and denitrification methods (anoxic reduction of $\text{NO}_3\text{-N}$ to N_2). Simultaneous nitrification-denitrification process (SND), in compare to conventional biological nitrogen removal process, can offer several advantages including reducing carbon source and alkalinity consumption, low energy consumption, high nutrients removal efficiencies, and simplifying the treatment system. P removal is achieved through Enhanced Biological Phosphorus Removal (EBPR) under alternating anaerobic-aerobic conditions. Biological nutrient removal (N and P) in batch anoxic experiments was investigated. The initial concentration of P and N were 10-18 mg $\text{PO}_4\text{-P/L}$ and 48 ± 2 mg $\text{NH}_4\text{-N/L}$. Sodium acetate was used as carbon source, at C/N 1 to C/N 7. Results indicated that the increase of C/N ratio improved efficiency of N removal in a range from 14.3 % at C/N 1 to 89,7 % at C/N 7. And also, the highest P removal of 61% was achieved at C/N 4. Nutrient removal was achieved by simultaneous nitrification and denitrification, and phosphorus removal.

Biography

Tea Širac graduated from Faculty of Food Technology and Biotechnology at the University of Zagreb in 2016. She is a Master of Molecular Biotechnology. From 2017, she has been working at Faculty of Food Technology and Biotechnology as a Scientific Assistant in a Laboratory for the Biological Wastewater Treatment. Tea has been participant at IWA MEWE 2016 in the field of Microbial ecology in aerobic granular sludge processes, and at 16th Ružička days within the topic: Environmental Protection.

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Numerical and experimental investigation of mixture uniformity and predicted performance of Urea-SCR system with vanadium-based catalysts based NH₃-Temperature programming desorption experiment

Changhee LEE and Hyeonku PARK
Songwon University, South Korea

The SCR technology for the control of NO_x emission from Marine Diesel engine was brought to the IMO Tier 3 regulation for marine diesel engine applications. SCR system is effective over a wide temperature region to reduce NO_x emission from engine exhaust emission during rich and lean operations. In this paper, SCR catalyst of V₂O₅-WO₃/TiO₂ is investigated and modeled. A global ammonia SCR reaction mechanism has been used, kinetic parameters for SCR system of NO_x by Urea was developed for V₂O₅-WO₃/TiO₂ SCR catalysts. The kinetic analysis was carried out using a commercial one-dimensional aftertreatment code, coupled with an optimizer. In this paper, the development of a steady kinetic model of the Urea-SCR process for vanadium-based catalysts is presented. The model was based on the results from reactivity, chemistry, catalytic mechanism, and kinetics of NH₃-TPD, NH₃ oxidation, NO oxidation, NO: NO₂ ratio, space velocity and NH₃/NO_x ratio over a commercial V₂O₅-WO₃/TiO₂ catalyst performed in our laboratories.

Biography

Changhee LEE completed his PhD at the age of 35 years from Hanyang University and postdoctoral studies from OKAYAMA University School of Mechanical engineering. He is the professor of Songwon University in Korea. He has published more than 45 papers in reputed journals and has been serving as a member of repute.

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Effect of the sprinkler irrigation on the space-time dynamic of translocation of As and Cd in the system soil – rice as a function of the pollution level of the soil

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Among the factors affecting the bioaccumulation of As and Cd in rice, a key role is played by the nature of irrigation methods. The sprinkler irrigation method, optimized for rice in Sardinia, Italy, applied to several rice genotypes over a number of crop years has produced no significant differences in yields, exhibiting also a number of environment-friendly features. In addition, our studies show that the adoption of sprinkler irrigation causes, in comparison to data obtained from rice grain irrigated by traditional irrigation method, an extraordinary As reduction (ca. -98%) and a meaningful Cd reduction (-20%) on rice grains. Since our previous experiments were accomplished on unpolluted soils, the aim of this study was to verify if the sprinkler irrigation is able to mitigate the bioaccumulation of both elements in rice grain cultivated also in soils heavily polluted by As and/or by Cd. Rice genotype (Carnise) has been cultivated using sprinkler irrigation in four soils at different pollution levels by As and Cd (up to 60 mg/Kg each). Beyond As and Cd, also the amounts of Cr, Cu, Hg, Mo, Mn, Ni, Pb, Se, Tl and Zn have been measured by ICPMS, GFAAS and FAAS techniques, along five different phenological phases, in soils and different parts of rice plant. Sprinkler irrigation allowed to obtain - also on heavily polluted soils from As and Cd - rice grain with concentration of such elements largely below the limits set for them by EFSA and EC (0.2 mg/Kg for both elements).

Biography

Gavino Sanna is Associate Professor of Analytical Chemistry at the Department of Chemistry and Pharmacy, University of Sassari, Italy. Scientific interests in chromatography, ICPMS, electroanalysis, food chemistry and analysis, environmental monitoring and analysis, role of the irrigation techniques in the bioaccumulation phenomena of toxic elements in rice. Reviewer of many tens of Journals of Analytical Chemistry, Food Chemistry, Environmental Chemistry. Enrolled in the Editorial Board of Analytics, SM Analytical and Bioanalytical Techniques and Advances in Food Science and Engineering. Author of ca. 200 among papers, patents and communications.

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Chemical composition of PM10 collected at workplace atmosphere in an iron foundry

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In the last, the industrial sector has been revitalized in Cuba. Specifically, the metal-mechanical industry has been extensively used to produce parts for the sugar industry, iron and steel industry as well as other industries. Former iron and steel work sites are significant in terms of their degree of pollution. The aim of this research was to determine the elemental composition of PM10 and water soluble ions associated to this particle fraction at workplace atmosphere in an iron foundry. The PM10 was sampled by a low volume sampler and PM10 concentrations were collected using a filter paper. The sampling was made during the process of molding, unmolding, and casting of iron and non-working days. The samples collected were analyzed by the energy dispersive X-ray fluorescence technique. In the excitation, an X-ray tube of Gd operated at 6 mA/100 kV/1500 s, 8 mA/75 kV/1500 s and 17.1 mA/35 kV/840 s irradiated secondary targets of Mo, Ge and Ti respectively. The ionic species were analyzed by ion chromatography. The results show that the highest concentrations are for Na, Mg, Al Si, S, Cl, K Ca, Fe, Cu Zn, Sn and Pb. There are elements such as P, Ga, Ge, As, Se, Rb, Y, Zr, Cd, I, Cs and Ba whose concentration levels were below the limit of detection and the blank limit of detection during all processes. Thirteen ions were analyzed but, only Na⁺, Mg²⁺, Ca²⁺, Cl⁻, NO₃⁻, and SO₄²⁻ were found. The highest values were found during working days, although in some cases the levels are also high during non-working days.

Biography

Daniellys Alejo Sánchez has completed her PhD from Antwerp University. She is the Director of the RIP project "Characterization and analysis of particulate compounds in multiple workplace atmospheres" developed between the University of Antwerp and the Universidad Central "Marta Abreu" de las Villas. She has published some papers in reputed journals and has been serving as a reviewer of several papers.

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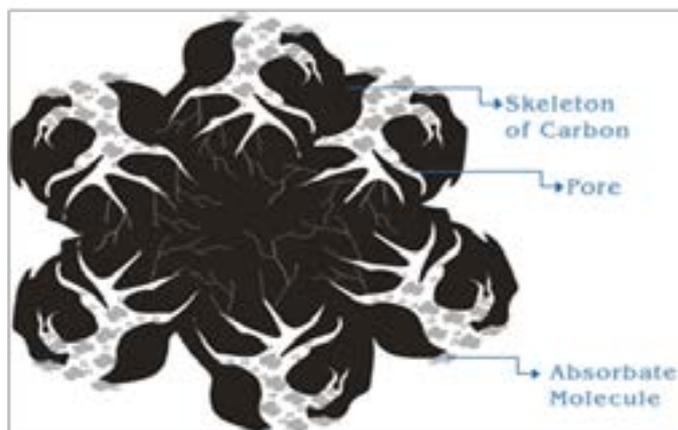
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Green activated carbons for mercury removal

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Activated carbons are considered to be the most successful adsorbent materials due to their high adsorption capacity for the majority of pollutants (dyes, heavy metals, pharmaceuticals, phenols, etc). They possess large surface area, and different surface functional groups, which include carboxyl, carbonyl, phenol, quinone, lactone and other groups bound to the edges of the graphite-like layers. Therefore, they are regarded as good adsorbents both in liquid and gas phases. The most widely used carbonaceous materials for the industrial production of activated carbons are coal, wood and coconut shell. These types of precursors are quite expensive and often imported, in many places; hence making it necessary, particularly for developing countries, to find a cheap and available feedstock for the preparation of activated carbon for use in industry, drinking water purification and wastewater treatment. In order to reduce the synthesis cost of activated carbons, some green final products are recently proposed, using several suitable agricultural by-products (lignocellulosics) - i.e. including olive-waste cakes, cattle-manure compost, bamboo materials, apple pulp, potato peel - as activated carbon precursors. In this work, special attention is given to those activated carbons (synthesis, and adsorption applications) which can be characterized as “green” because their origin are green environmental-friendly sources. The application of the prepared carbons was for mercury removal from aqueous solutions.



Biography

George Z Kyzas obtained his BSc, MSc and PhD degrees at Aristotle University of Thessaloniki (Greece). His current interests include the synthesis of various adsorbent materials for the treatment of wastewaters (dyes, heavy metals, pharmaceuticals, phenols, etc). He has published significant scientific papers, books (as Author and/or Editor), chapters in books, teaching notes and reports. He also acted as Guest Editor in Special issues of journals and presented many works in international conferences. He has been awarded with honors, grants and fellowships for his research career/profile by (i) Research Committee of Aristotle University of Thessaloniki (2009, 2013), (ii) National State Scholarships Foundation of Greece (2013) and (iii) Stavros Niarchos Foundation (2016).

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Analysis of absorption heat pump in parallel flow powered by the biogas

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The energy crisis and the environmental problems have focused the researchers on absorption heat pumps [1]. In this research, a sensitivity analysis is carried out for a double effect absorption heat pump in parallel flow powered by biogas, using ChemCad software. The system uses 350 kg/h of LiBr-H₂O working fluid at 56 % w/w to avoid crystallization phenomena. The cycle is involved between the absorber and sub-cooling condenser temperature equal to 277 K and 310 K respectively. In this heat pump with two levels, the condensation heat in the higher-pressure generator is used in a lower pressure generator. The study is developed varying the temperature of the higher-pressure generator. Results show that this parameter has a negative effect on the coefficient of performance (COP). Lower pressure in the higher-pressure generator could increase the COP, but determines lower pressure in the lower-pressure generator and in the condenser. In this condition, the heat pump needs of a refrigerant solution with very low temperature in the condenser, making the choice unattainable. For this reason, it is necessary to avoid high value of COP. The temperature of the higher-pressure generator has also a negative effect on the cooling capacity, because the pressure difference between the condenser and evaporator increases, increasing the feeded steam and then reducing the cooling power. The analyzed factor has a positive effect on the heat exchanged in the two generators, because the heat needed to the evaporation increases. The temperature of the higher-pressure generator has a negative effect on the heat exchanged in the condenser, because increasing the condensation temperature the latent heat decreases. The heat transferred to economizers and their efficiency increase with the maximum cycle temperature especially for the low temperature economizer. Future researches should optimize the system considering the efficiency and the costs.

Biography

Grazia Leonzio is a PhD student from L'Aquila University. She published several articles and participated to several international and national congresses about environmental and energy aspect of chemical processes. She wrote an article about waste management in Italian regions and published in Columbia University web-side. She participated to M.U.N conferences and she is a member of several associations: A.I.D.I.C. (Italian Association of Chemical Engineering), S.C.I. (Italian Chemical Society), I.S.S.N.A.F. (Italian Scientists and Scholars in North America), E.C.A.S. (European Commission Authentication Service). She is a referee of several journals.

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Physicochemical and bacteriological analyses of water samples from hand dug wells in Lafia metropolis, Nasarawa State, Nigeria

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This study investigated the physicochemical parameters and bacteriological quality in hand dug wells in Lafia metropolis of Nasarawa State. A total of five selected hand dug wells samples were analyzed using standard methods. The observed physicochemical parameters were temperature, pH, electrical conductivity, total hardness, total dissolved solid (TDS), total suspended solid (TSS), total solid (TS), nitrate NO_3^- , phosphate PO_4^{3-} and chloride (Cl^-). The results of the physicochemical parameters ranged as follows: Temperature (28-30°C), pH (4.71-6.85), conductivity (28-825 $\mu\text{s}/\text{cm}$), total hardness (45-78 mg/L), TDS (18-550 mg/L), TSS (0-490 mg/L), Cl^- (10.77-79.85 mg/L), NO_3^- (143.66-656.44 mg/L) and PO_4^{3-} (0.271-7.4 mg/L). NO_3^- in water exceeds the WHO standard for drinking water, parameters such as total hardness, total dissolved solid, total suspended solid, total solid, chloride, and electrical conductivity had some sample exceeding the WHO standard while others were below the WHO standard. The bacteriological analysis carried out on the water shows that, none of the samples complied with bacteriological standards as total aerobic counts, generally exceeded permissible limit of 100 CFU/ml for coliform count and 1.0×10^2 CFU/ml for bacteria and pathogen count such as *Escherichia coli*, *Pseudomonas aeruginosa*, *Staphylococcus aureus*, *Staphylococcus* spp., *Serratia marcescens*, *Proteus* spp. and *Micrococcus* spp. counts were very high.

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Artificial photosynthesis to convert CO₂ into solar fuels: Can we do better than Mother Nature?

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Finding effective ways for conversion of CO₂ into hydrocarbons (as energy fuels or chemical feedstock) is highly desirable to achieve sustainable development. Artificial photocatalytic conversion of CO₂ to hydrocarbons such as methanol makes possible simultaneous solar energy harvesting and CO₂ reduction, two birds with one stone for the energy and environmental issues. In this talk, I will overview the current status in artificial photosynthesis and present our progress in green processing of earth-abundant and environment-friendly semiconductors to achieve the goal. In our attempt, modified graphene oxides (GOs) has been utilized to prove the concept and showed 4 times enhancement in activity over a commercial TiO₂ (P25). Further modification including copper nanoparticle addition to form hybrids to achieve 60 times enhancement in catalytic activity has been demonstrated. On the other hand, a SnS₂ with carbon addition yield quantum efficiency up to 0.7% to convert CO₂ into acetaldehyde, which is highly valuable in polymer industry. The conversion efficiency is comparable to that of photosynthesis in nature and sheds light for a brighter future. Detailed preparation, characterization, and performance of the catalysts will be presented. The role and interplay of the constituent components will also be discussed.

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Replacing Pd(OAc)₂ with supported palladium nanoparticles in C-H bond, C-O bond activation reaction

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Supported palladium nanoparticles were used as an efficient catalyst for C-H bond, C-O bond activation reaction for the synthesis of aromatic ketones, amides and quinones. The catalyst can be reused for five cycles without significantly losing activity. The XPS analysis of the catalyst before and after reaction suggested that the reaction might be performed via a catalytic cycle that began with Pd⁰. The hot filtration test strongly suggests that the present reaction would proceed via heterogeneous manner.

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Promotion and implementation of bioenergy for a better environment: A mini review

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Biogas from biomass appears to have potential as an alternative energy source, which is potentially rich in biomass resources. This is an overview of some salient points and perspectives of biogas technology. The current literature is reviewed regarding the ecological, social, cultural and economic impacts of biogas technology. This article gives an overview of present and future use of biomass as an industrial feedstock for production of fuels, chemicals and other materials. However, to be truly competitive in an open market situation, higher value products are required. Results suggest that biogas technology must be encouraged, promoted, invested, implemented, and demonstrated, but especially in remote rural areas. (1) Biogas technology can not only provide fuel, but is also important for comprehensive utilisation of biomass forestry, animal husbandry, fishery, evolving the agricultural economy, protecting the environment, realizing agricultural recycling, as well as improving the sanitary conditions, in rural areas. (2) The biomass energy, one of the important options, which might gradually replace the oil in facing the increased demand for oil and may be an advanced period in this century. Any country can depend on the biomass energy to satisfy part of local consumption. (3) Development of biogas technology is a vital component of alternative rural energy programme, whose potential is yet to be exploited. A concerted effect is required by all if this is to be realised. The technology will find ready use in domestic, farming, and small-scale industrial applications. (4) Support biomass research and exchange experiences with countries that are advanced in this field. In the meantime, the biomass energy can help to save exhausting the oil wealth. (5) The diminishing agricultural land may hamper biogas energy development but appropriate technological and resource management techniques will offset the effects.

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Solvent selection guides for pharmaceutical chemistry

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As solvents represent most of the material used to produce an Active Pharmaceutical Ingredient, selecting the "greenest" solvents and reducing their amount is the most effective way to improve the sustainability of its synthesis. Several solvent selection guides have been published by pharmaceutical companies or institutions (Pfizer, GSK, GCI-PR, and Sanofi). A special focus on Sanofi's guide will be made. As part of the European project CHEM21, a survey of these solvent guides has been made, permitting to rank many classical solvents into four categories, from "recommended" to "highly hazardous". In order to rank less classical solvents, and in particular bio-derived solvents, a methodology has been developed. A set of Safety, Health and Environment scores is proposed, based on very easily available physical properties and GHS statements. A simple combination of these scores gives a preliminary ranking of any solvent. The CHEM21 solvent selection guide thus obtained is the first guide integrating bio-derived solvents. The guide and the methodology have been integrated in the CHEM21 on-line training platform, which is publically available. A demonstration of this platform will be made.

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Codisplay of diisopropyl-fluorophosphatase (dfpase) and organophosphorus acid anhydrolase (opaa) enzymes in cell surface of e.coli

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Backgrounds: Pesticides used in controlling harmful populations of insects, can adversely affect human health and cause environmental pollution. The most popular pesticides are organophosphates (OPs) such as Diazinon, Chlorpyrifos, Malathion, etc. Several enzymes have been isolated able to degrade different kinds of OPs such as OPAA (from cytoplasm of *Alteromonas* sp.) and DFPase (from the brain of squid *Loligo vulgaris*). To reduce the OP uptake limitation and degrade a broader substrate spectrum with more activity, we demonstrate for the first time a functional codisplay of two distinct hydrolases, DFPase and OPAA, on a single bacterial cell, by fusing each enzyme to N-terminal of InaV (InaV-N).

Materials and Methods: To cotranslocate, target genes should be cloned in two different plasmids with two different antibiotic resistances and independent expression strategy, therefore, *inaV-N/dfpase* and *inaV-N/opaa* fragments were cloned into pET-28a(+) and pCDFDuet vectors, separately. Competent *E. coli* BL21 cells were transformed by individual recombinant plasmids, as controls, and simultaneously both one by electroporation method.

Results: Studies on activity by FPLC with DFPase, OPAA and codisplay cells showed a specific activity of 19.676, 13.125 and 22.46 U/ml, respectively, for Diazinon, and 10.779, 5.213 and 13.784 U/ml, respectively, for Chlorpyrifos. Study on activity by monitoring fluoride-release from DFP by each miligram of DFPase, OPAA and codisplay wet cells showed 500, 250 and 800 Unit, respectively.

Discussion: Findings showed a recombinant strain possesses a broader substrate spectrum and a more activity than strains expressing either one of the hydrolases, a whole-cell biocatalyst candidate to detoxify environment polluted by different OPs.

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Electrochemical reactor design/fabrication for CO₂ electroreduction to low-carbon fuels/chemicals

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Extra emission of carbon dioxide (CO₂) into the atmosphere, induced by human industrial activities, has been considered one of the primary causes in possible global warming due to the greenhouse effect, and also becoming an increasing concern in recent years. To address this issue, using electrochemical reduction to convert CO₂ to useful small fuels such as CH₄, CH₃OH, HCOOH, C₂H₂, etc., represents a value-added approach to the simultaneous generation of alternative fuels and environmental remediation of carbon emissions from the continued use of conventional fuels. Many references in the literature have focused on studies with improving the performance of electrochemical process to convert CO₂ into low-carbon fuels/chemicals. For reactor components, both anodes and cathodes are discussed in terms of their materials, structure, design, fabrication, as well as their effects on the reactor's performance and productivity. Several important electrodes are described including metallic electrodes, gas diffusion electrodes (GDEs) and modified metal electrodes in both aqueous and non-aqueous electrolyte solutions. Both the ion-exchange membranes for low-temperature operation, and the solid oxide electrolyte layers for high-temperature operation, can serve as both functions of ion conduction and electrode separating. Regarding the electrochemical reactor design/assembling/fabrication for CO₂ reduction, several types of the reactors, including the conventional three-electrode cells, the low temperature two-electrode cells using proton exchange membrane fuel cell (PEMFC) technology, the solid oxide electrolysis cells (SOECs) and the microbial electrolysis cells (MECs), as well as other electrolysis cells, are introduced and their performances are also analyzed. The potential and feasibility of the reactor scale-up for CO₂ conversion to low-carbon fuels/chemicals is discussed with respect to the technology's commercialization.

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Green synthetic route to access functionalized bio-active organic scaffolds using tetragonal nano-ZrO₂ as reusable solid acid catalyst

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Over past decades, one-pot multicomponent reactions (MCRs) have been established as one of the important synthetic tool for the synthesis of bio-active organic scaffolds. As a part of our interest to develop green and efficient multicomponent protocol, we have demonstrated the role of nanoparticles (NPs) in MCRs in determining the selectivity and performance of the protocol. In this presentation, the role of ZrO₂ NPs in one-pot MCRs leading to fabrication of bio-active organic moieties such as, benzylpyrazolyl coumarin (I), pyrano[2,3-c]pyrazole (II), coumarin fused 4*H*-chromene (III) and 2-amino-chromene (IV), derivatives will be presented. In addition, the effect of phase (tetragonal/monoclinic/cubic), surface defect and size of the NPs as well as effect of solvent on the rate of the reaction will be discussed. We observed that the ZrO₂ NPs can be recycled up to ten times without any notable change in catalytic activity and morphology.

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Mechanochemical synthesis of functional pharmaceutical solids

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This is an exciting time for mechanochemistry: vast progress has been made in the last three decades, especially in academic research, and new areas of applications of such green technology will soon impact substantially in real world applications. With specific regard to pharmaceutical materials, the design of functional molecular solids has advanced tremendously through mechanochemistry. However, mechanochemistry is often performed somewhat superficially, while a good routine screening of new solid forms requires covering a wide crystallization space by using different experimental conditions. This presentation provides an overview of advances in the synthesis of new pharmaceutical forms, which have been provided through mechanochemical methods. Such techniques are able to cover a wide range of crystallization space thereby increasing the probability of discovering different crystalline forms.

Liquid-assisted grinding (LAG) remains the most explored mechanochemical technique for the synthesis of new pharmaceutical solid forms and its higher efficiency for generating new multicomponent solids has been demonstrated: the properties of the “catalyst” are of paramount importance for the discovery of new polymorphic forms. The most recent version of variable-amount LAG (VALAG) will possibly contribute to the development of practical methods for polymorph screening and selection of a proper liquid to industrially produce (via solution crystallization) the desired polymorphic form. Polymer-assisted grinding (POLAG) also represents a new efficient mechanochemical technique for the synthesis and screening of new solid forms. This method in particular eliminates the risk of by-products such as solvates during polymorph, salt and cocrystal screening. Other interesting, yet not explored, combinations of mechanochemical methods will be proposed. Overall, mechanochemistry should not be considered simply as an alternative method but rather as a key strategy in any fully effective solid form screen with reduced effort and time as well as the potential of requiring reduced amounts of available material.

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Development in biological conversion process of carbon dioxide from industrial flue gas to microalgae biomass

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Biological conversion of CO₂ using microalgae can be a sustainable solution to address global warming and energy crisis caused by fossil fuels. Microalgae have attracted considerable attention due to their ability for production of biofuels and useful chemicals by photosynthesis, and it is promising agent for biological CCU (carbon capture and utilization) technology. We developed two-track approach for effective microalgal CCU technology; first one is development in various micro-scale screening technology using microfluidic devices to select highly productive strain. Second one is development in mass culture system directly using the industrial flue gases. Flue gas containing 3–5% CO₂ from the combustion of LNG (liquefied natural gas) in CHP (combined heat and power) plants was supplied as carbon-feedstock to produce microalgae biomass. In the present system, natural solar radiation and hot water that has been heated without consuming any electric power were also used to improve the economic feasibility of CO₂ capture from the flue gas using microalgae. Also, blower was continuously operated from the stack of power plant to microalgae cultivation site to supply the flue gas. In addition, we developed a low-cost thin-film photobioreactor (PBR) system with a vertical bubble column, which can provide a viable option for direct capture and utilization of concentrated CO₂ emitted from power plants due to usability of scale-up and efficient capture of CO₂. Demonstration of biological CCU process was improved by integrating these technologies.

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SpecSoil: The newest innovative green technology for soil analysis

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A new methodology for soil analysis fertility based on the use of vibrational spectroscopy and Chemometrics has been developed and validated. This methodology employs Near Infrared Spectroscopy (NIRS) and multivariate calibration for the quantification of several soil fertility attributes such as Soil Organic Matter (SOM), silt, clay and sand. Current methods for evaluating these parameters are still based on wet chemistry methods which are time consuming and also generate residues that require additional treatment to be disposed of in nature. Due to the growth of precise agriculture there is a huge demand for analytical methods that can provide simple, fast, environmentally friendly and precise diagnosis for soil fertility. The growing interest in NIRS technology can be justified by the numerous and remarkable benefits that NIRS spectroscopy offers over conventional analysis: (i) it is a non-destructive technique, (ii) it is free from undesirable residues and thus has minimal environmental impact, (iii) it is a low-cost technique and (iv) it is a rapid and innovative technique that requires little sample handling when combined with Chemometrics. In this lecture, the methodology which is based on a huge spectral and analytical soil data bank representative of the Brazilian territory will be presented.

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Properties of green solvents and their applications in green chemistry

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Many conventional chemical processes result in environmental pollution and are unsustainable. Green chemistry is the future of chemistry and chemical industry. Effective utilization of green solvents, such as water, supercritical fluids (SCFs), ionic liquids (ILs), liquid polymers, switchable solvents is an important area of green chemistry. The use of green solvents provides additional control factors for optimizing different chemical processes. Recently, much attention has been paid to the properties and applications of green solvents in extraction and fractionation, chemical reactions, and material synthesis. Many processes that use green solvents have been commercialized. The field of green solvents has a very bright future and there are many challenges from both fundamental and practical point of view. In recent years, we are very interested in physicochemical properties of green solvents and their applications in green chemistry, which include mainly: 1) phase behavior, intermolecular molecular interaction, and the microstructures in complex SCFs, ILs, supercritical (SC) CO₂/IL systems; 2) colloid and interface science of green solvent systems, including chemical thermodynamics, microstructures, and functions; 3) effects of phase behavior and intermolecular interactions on the properties of chemical reactions in SC CO₂, ILs, SC CO₂/water, water/ILs, and SC CO₂/ILs; 4) synthesis of highly efficient catalytic materials using green solvents; 5) development of greener routes for the transformation of CO₂, biomass and aromatics into value-added chemicals in green solvents, and the optimization of the reaction processes using the designable and tunable features of green solvents. In this presentation, I would like to discuss some recent results.

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Carbon fibers from plant-derived material

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Because of the Kyoto protocols on CO₂ emission reduction, the transition towards a bio-based economy and sustainable developments offers high perspectives for natural fibers markets. Several kinds of natural fibers exist around the world: bamboo in Japan, coconut in equatorial countries. They are supposed to be one of the strongest natural fibers available in nature. Biochar based carbon and graphene nanostructures are very perspective raw materials for nano profiling and nano-modification of composites for the promising applications in material industry. Considering continues, growing global carbon fibers (CFs) demand various applications, investigation of the possibility to use the natural fibers to carbon fibers studied. Pyrolysis method was adopted for conversion. The aim of the study was to use affordable, easily available, environment-friendly material to produce carbon fibers. These carbon fibers may become, in perspective, substitutes for traditional polymeric precursors for CFs. Carbonized Fibers were studied by FESEM, Raman and TGA. Various applications like the mechanical strength of composite were studied further. Results show that biochar based carbon fibers prove themselves as potential fillers in composite.

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Lignin into aromatics: Bridging homogeneous and heterogeneous catalysis

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The development of efficient catalytic conversion of lignin into aromatic chemicals remains an important challenge in catalysis due to the amorphous carbon-based inactive property and highly heterogeneous nature of lignin. Potential strategies for the production of aromatics from lignin need to address the issues of lignin solubility as well as of the selective cleavage of the aryl ether bonds. In this lecture, we will discuss our progress in catalytic lignin valorization relating to aforementioned two aspects. In the first part, we will report the selective cleavage of aryl ether in lignin to afford monophenols over tungsten carbide (W_2C) catalysts. The activation mechanisms of different aryl ether bonds over W_2C are deeply explored. On the other hand, synergistic effect between W_2C and a second metal, the effect of the monomer structure on the catalytic performance, and the catalyst stability under liquid phase conditions will be discussed as well. In the second part, selective cleavage of lignin to aromatic compounds catalyzed by methyltrioxorhenium (MTO) without any oxidant (e.g. H_2O_2) and reducing agent (e.g. H_2) is proposed. The introduction of ionic liquids supplies a homogeneous platform which allows the process conducting under mild condition. Microwave irradiation could accelerate the reaction rate and significantly increase the activity. Under optimized conditions, a series of lignin β -O-4 model compounds could afford guaiacol as the primary product with the yields higher than 67%. The possible mechanisms for degradation of lignin is proposed based on IR spectroscopy and NMR results.

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Designing green catalysts using earth-abundant metals: solving the “how-to” and “why” questions using quantum chemistry approaches

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It is a general challenge to design highly active or selective green catalysts using earth-abundant metals. We demonstrated an effective computational approach to deterministically search for optimal binding sites on Cu (100) surface (for catalytic hydrogenation) through the doping of Fe and/or Zn using the inverse molecular design methods. A stable Zn-doped Cu (100) surface was found with optimal binding affinity to H-atoms. We understood the electronic structure cause of the optimal binding sites using orbital-specific binding energy analysis, a new quantum chemistry analysis method here. Overall, we found that the Zn atomic orbitals show less participation in the binding event of H-atoms than the Cu atomic orbitals. In particular, compared to the 3d-orbitals of surface Cu atoms, the 3d-orbitals of surface Zn-atoms show less binding energy contribution and participation, and are much less influenced by the electronic couplings of the media Cu atoms. Our study provides valuable green chemistry insights for the design of green catalysts using earth-abundant metals. Our designed Cu-based earth-abundant alloys may be used for important catalytic hydrogenation applications such as lignin degradation or CO_2 transformation.

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Green energy potential of plant biomass and natural biopolymers

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Nowadays the main energy sources (over 80%) are fossil fuels, namely coal, petroleum and natural gas. The increased use of the fossil fuels is causing acute environmental problems, since emission of carbon dioxide in the volume of 1500-2000 m³ per 1 ton of fuel, triggering the greenhouse effect and global warming of the Earth. Therefore, in recent years, a considerable attention is paid to the production of the green energy from plant biomass, which in contrast to fossil energy sources is neutral for emission of carbon dioxide. Furthermore, the biomass is continuously renewed in the nature as a result of the photosynthesis. Various biomass types involve residues of forest and agricultural plants; residues and waste of textile, pulp and paper industry; municipal paper waste; special energy crops; etc. The total amount of such biomass type that is accumulated annually in the world is estimated to be 10-15 billion tons at least. Currently, the share of biomass-based energy is about 10-12% in the world. The complete use of all energetic potential of non-edible plant biomass can increase the share of the green energy to 30-33% in the world energy consumption. It is known that the plant biomass is a composition of three main biopolymers – cellulose, hemicellulose and lignin, as well as small admixtures of some other components such as protein, pectin, starch, rosin acids, waxes, fats, minerals, etc. Thus, to obtain the net combustion heat of the biomass sample (q), a net heating value (q_i) of the individual component and its weight part (w_i) in the biomass should be summarized: $q = \sum w_i q_i$. On the other hand, a quite precise equation can be derived for calculating the net heating value of the individual component with a low relative deviation up to 1%.

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Towards the selective formate production over nano-micro structured SnOx catalysts in aqueous medium

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In response to the fast consumption of fossil fuels and their associated environmental problems including the notorious greenhouse gas (CO₂), carbon capture and utilization (CCU) methods to convert CO₂ into value-added chemicals or fuels have aroused intense attention worldwide. Among these transformations, using electrochemical reduction to convert CO₂ to CH₄, CH₃OH, HCOOH, C₂H₂, etc. is particularly interesting as it could allow for intermittent and unpredictable renewable energy (i.e., solar or wind) to be stored in the form of these useful small fuels or chemical products. In the process of CO₂ electroreduction reaction (CER), slow kinetic and low production selectivity of CER are major challenges, leading to wastage of energy and the insufficient utilization of resources. Although some electrocatalysts are employed to accelerate the reaction kinetics and improve the selectivity, the processes of CER at the current state of technology are still not practical. Overcoming these challenges of CO₂ reduction under mild conditions would enable development of high efficient fuel-producing devices with practicability, especially for room-temperature CO₂ reduction in aqueous solutions. In view of these facts, we here report the design and synthesis of Sn oxides electrocatalysts with special 3D morphology including micropheric, coralline-like and flower-like structure by simple hydrothermal method. All of these SnOx catalysts were coated on the gas diffusion carbon paper sheets to form target electrodes. To our interesting, all the obtained SnOx exhibited the superb CER catalytic activity and selectivity toward formate production with FE% > 60%, but the electrode modified with coralline-like structured SnOx is more efficient due to its exposed more {002} planes of SnO₂ with FE% reaching to 87%.

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Factors affecting seawater-based pretreatment of date palm residues for bioethanol production

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The utilization of seawater in biorefinery has gained increasing interest recently. Seawater-based pretreatment of lignocellulosic biomass as an innovative approach has been demonstrated in our previous study 1. With respect to process optimization, factors affecting seawater-based pretreatment of lignocellulosic date palm residues were studied for the first time in this paper. Pretreatment temperature (180°C-210°C), salinity of seawater (0ppt-50 ppt), and catalytic chemicals (H₂SO₄, Na₂CO₃, and NaOH) were investigated. The results showed that pretreatment temperature exerted the largest influence to seawater-based pretreatment in terms of the enzymatic digestibility (ED) (t Ratio = 20.398) and fermentability (FB) (t Ratio = 36.861) of pretreated solids, and the inhibition of pretreatment liquids to *Saccharomyces cerevisiae*. Though salinity brought the least effects (t Ratio is 0.449 for ED and is -0.359 for FB) to seawater-based pretreatment, the independence on salinity widens the spectrum of saline water sources including not only seawater but also brines discharged after desalination. Sulfuric acid (t Ratio is 9.09 for ED and is 13.83 for FB) was the most effective catalytic chemical for seawater-based pretreatment compared with Na₂CO₃ (t Ratio is -5.55 for ED and is -7.02 for FB) and NaOH (t Ratio is -4.91 for ED and is -7.68 for FB) as shown in our study. Statement of the Problem: Women who have experienced intimate partner violence (IPV) are at greater risk for physical and mental health problems including posttraumatic stress disorder (PTSD) and alcohol dependency. On their own IPV, PTSD and alcohol dependency result in significant personal, social and economic cost and the impact of all three may compound these costs. Researchers have reported that women with these experiences are more difficult to treat; many do not access treatment and those who do, frequently do not stay because of difficulty maintaining helping relationships. However, these women's perspective has not been previously studied. The purpose of this study is to describe the experience of seeking help for alcohol dependency by women with PTSD and a history of IPV in the context in which it occurs. Methodology & Theoretical Orientation: An inter subjective ethnographic study using hermeneutic dialogue was utilized during participant observation, in-depth interviews and focus groups. An ecological framework was utilized to focus on the interaction between the counselors and the staff to understand this relationship and the context in which it occurs. Findings: The women in this study were very active help seekers. They encountered many gaps in continuity of care including discharge because of relapse. Although the treatment center was a warm, healing and spiritual place, the women left the center without treatment for their trauma needs and many without any referral to address these outstanding issues. Conclusion & Significance: Women with alcohol dependence and PTSD with a history of IPV want help however the health and social services do not always recognize their calls for help or their symptoms of distress. Recommendations are made for treatment centers to become trauma-informed that would help this recognition.

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Greener approach to prepare electrospun antibacterial β -cyclodextrin-based nanofibers for removal of bacteria from water

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Statement of the Problem: Water in Southern Africa is becoming a lot scarcer and the quality can be poor, especially in rural communities where there is no access to purified tap water. As a result, the impact of water-borne diseases is significant. The lack of water has resulted into conflicts and protests in some communities. Groundwater from boreholes and wells plays an important role in water supply, but due to limited hydrological knowledge, these drinking water sources are not always well-designed and they are prone to contamination. Poor sanitation is another problem; e.g. it is well-known that nearby located latrines can result in fecal (and thus pathogenic) contamination of open wells and boreholes. The aim of this project was to develop viable sustainable solutions that involved the integration of nanofibers to a filtration system.

Methodology & Theoretical Orientation: Electrospun nanofibres containing Ag⁺/Fe³⁺ ions were subjected to UV-reduction in the presence of water vapor created in a unique system under inert atmosphere at temperatures below 100°C to reduce the ions to zero-valent state, thus avoiding the use of other toxic reducing agents such as ammonia.

Findings: The average diameter of the β -CD-based nanofibers was 382.12 \pm 30.09 nm and that the diameters of Ag and Ag/Fe NPs were 38.81 \pm 8.21 nm and 56.29 \pm 12.64 nm, respectively, after reduction. The effect of UV irradiation time on the reduction of the Ag⁺ and Fe³⁺ was studied by measuring the UV-vis absorbance of the reduced NPs. The Ag and Ag/Fe NPs embedded on the β -CD-based nanofibers exhibited a strong biocidal effect on all of the bacteria strains.

Conclusion & Significance: The nanofibers were also tested on real water samples and were found to be effective in killing bacteria in the water.

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Efficient and selective palladium-catalyzed telomerization of 1,3-butadiene with carbon dioxide

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The sustainable approaches for the synthesis of value-added fine and bulk chemicals using viable raw materials and feed stock has been accepted as a collective knowledge by our society. From the aspect of organic syntheses, the development of chemical reactions, with high atom efficiency is the main targets. In this respect, carbon dioxide is considered as a valuable C1 building block due to its abundance, low toxicity and recyclability. To create essential C-C bonds from CO₂ using traditional synthetic methodologies, the use of strong carbon nucleophiles is necessary, which also generate stoichiometric amounts of by-products. In contrast, the catalytic telomerization of 1,3-butadiene with carbon dioxide leads to the unsaturated δ -lactone (3-ethylidene-6-vinyltetrahydro-2H-pyran-2-one) under mild conditions in a 100% atom-efficient manner. Herein, we report our finding on improved palladium catalyst systems for the telomerization of 1,3-butadiene with carbon dioxide and also report the first related reactions with 1,2-butadiene.

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