PEERS ALLEY MEDIA

4TH EDITION OF

ADVANCED CHEMISTRY WORLD CONGRESS

MARCH 27-28, 2023

BARCELONA, SPAIN

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ADV. CHEMISTRY 2023

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PROGRAM-AT-A-GLANCE

ADV. CHEMISTRY

2023

DAY 1

MARCH 27, 2023

Scientific Program

08:00-09:00	**Registrations**
09:00-09:30	**Opening Ceremony**

Moderator: Dimitrios Kotzias, *Institute for Health and Consumer Protection, Italy*

Keynote Forum 09:30-11:00

09:30-10:00	**Title: Naturally occurring radioactive materials in oil exploration: How did this happen?** **Sheldon Landsberger,** *University of Texas at Austin, USA*
10:00-10:30	**Title: Aerosol collector addition in coarse particle flotation** **Liza Forbes,** *University of Queensland, Australia*
10:30-11:00	**Title: Design of agonists for the selective activation of BMP signalling using the three-dimensional structure of BMP7 and a computer algorithm based on structure activity relationships and the physical chemical properties of amino acids** **William Carlson,** *Massachusetts General Hospital and Harvard Medical School, USA*

Networking & Refreshments 11:00-11:10

Session I (11:10-13:15) Distinguished Speaker Talks

Session Chair: Sheldon Landsberger, *University of Texas at Austin, USA*

11:10-11:35	**Title: Automated SEM/EDS analysis for assessment of trace cross-contamination in 316L stainless steel powders for additive manufacturing** **María José Balart Murria,** *University of Warwick, UK*
11:35-12:00	**Title: A decreased response to resistin in mononuclear leukocytes contributes to oxidative stress in nonalcoholic fatty liver disease** **Placida Baz,** *University of Buenos Aires, Argentina*
12:00-12:25	**Title: Subtle early-warning indicators of landfill subsurface thermal events** **Andy Davis,** *Geomega Inc, USA*

12:25-12:50	**Title: Total mandible and bilateral TMJ reconstruction combining a customized jaw implant with a free fibular flap** **Bruno Andrea Pesucci,** *Maxillo Facial Surgery Unit, San Camillo Forlanini Hospital, Italy*
12:50-13:15	**Title: Combination of Betulinic acid fragments and Carbonicanhydrase inhibitors – A new drug targeting approach** **Reinhard Paschke,** *Martin Luther University Halle-Wittenberg, Germany*

Group Photo

Lunch Break 13:15-14:00

Session II (14:00-15:40) Distinguished Speaker Talks

Session Chair: William Carlson, *Massachusetts General Hospital and Harvard Medical School, USA*

14:00-14:25	**Title: Consideration of net-zero concrete toward a carbon recycling society by a mineral carbonation using alkali wastes** **Yoshito Izumi,** *Sustainable Development Innovations, Japan*
14:25-14:50	**Title: Tailor-made alkaliphilic and thermostable fungal laccases for industrial wood processing** **Michael Lecourt,** *FCBA Institut Technologique, France*
14:50-15:15	**Title: Carbon dioxide (CO_2) utilization through chemical and electrochemical conversion** **Geoff Wang,** *The University of Queensland, Australia*
15:15-15:40	**Title: Water and its dielectric signature: New marker for biosensing** **Yuri Feldman,** *The Hebrew University of Jerusalem, Israel*

Networking & Refreshments 15:40-15:55

Session III (15:55-17:35) Distinguished Speaker Talks

Session Chair: Liza Forbes, *University of Queensland, Australia*

15:55-16:20	**Title: Direct optical measurement of corrosion layer thickness of archaeological lead artifacts; A new simpler dating method** **Sana Shilstein,** *Weizmann Institute of Science, Israel*

16:20-16:45	**Title: Chemical profile of tropical red wines from the Submiddle Sao Francisco Valley, Brazil** **Carlos Artur Alves,** *Centro Universitário Inta - Uninta, Brazil*
16:45-17:10	**Title: Orientation analysis of polymer thin films on metal surfaces via IR absorbance of the relative transition dipole moments** **Andreas Fruh,** *National Research Tomsk Polytechnic University, Russian Federation*
17:10-17:35	**Title: Developments of thermal protection materials in space missions and the current issues in this research** **Lars Pepermans,** *Netherlands*

End of Day 1

DAY 2

MARCH 28, 2023

Scientific Program

09:00-09:30	**Introduction**

Keynote Forum 09:30-11:00

09:30-10:00	**Title: Processing the ores of rare earth elements** **Terry McNulty,** *T.P. McNulty and Associates, Inc., USA*
10:00-10:30	**Title: HDAC inhibitors with non-hydroxamate warhead** **Franz-Josef Meyer-Almes,** *Darmstadt University of Applied Sciences, Germany*
10:30-11:00	**Title: Application of heterogeneous photocatalytic technology for the degradation of gaseous priority pollutants in ambient air and indoor environments** **Dimitrios Kotzias,** *Institute for Health and Consumer Protection, Italy*

Networking & Refreshments 11:00-11:10

Session IV (11:10-13:15) Distinguished Speaker Talks

Session Chair: Franz-Josef Meyer-Almes, *Darmstadt University of Applied Sciences, Germany*

11:10-11:35	**Title: From conventional to green: Latest trends in fertilizer industry** **Cemre Avsar,** *Toros Agri Industry and Trade Co. Inc, Turkey*
11:35-12:00	**Title: Synthesis and catalytic applications of metal complexes supported by NHC-based cyclophanes** **Daniel Mendoza-Espinosa,** *Universidad Autónoma del Estado de Hidalgo, Mexico*
12:00-12:25	**Title: Artificial intelligence applied to nutritional therapy in Moroccan type 2 diabetics: Methodological approach** **Saliha Chellak,** *Cadi Ayyad University, Morocco*
12:25-12:50	**Title: Lithium ions extraction from sea water bittern using room temperature ionic liquid** **Abdolreza Hormati,** *CEO Manager of the First Producer of Industrial Salt from Sea Water, Iran*
12:50-13:15	**Title: Preparation and characterization of PDMS-based antifouling coatings** **Esra Kasapgil,** *Izmir Bakircay University, Turkey*

Lunch Break 13:15-14:00

Session V (14:00-16:30) Distinguished Speaker Talks

Session Chair: Dimitrios Kotzias, *Institute for Health and Consumer Protection, Italy*

14:00-14:25	**Title: Structural and photoluminescence studies of microwave sintered Ce0.8Y0.1Dy0.1O2−δ solid electrolyte for IT-SOFC applications** **Ch Madhusudan,** *Government Degree College, India*
14:25-14:50	**Title: Eco-friendly synthesis and application of tin sulfide** **Asta Bronusiene,** *Kaunas University of Technology, Lithuania*
14:50-15:15	**Title: Selenium speciation analysis in lactic acid bacteria cultivated under stress conditions** **Vera Nesporova,** *University of Chemistry and Technology, Czech Republic*
15:15-15:40	**Title: Relationship among Blastocystis, the Firmicutes/Bacteroidetes ratio and chronic stress in Mexican university students** **Iliana Itzel Lozano-Ochoa,** *Universidad Juarez del Estado de Durango, Mexico*
15:40-16:05	**Title: Development of nimesulide analogs as a dual inhibitor targeting tubulin and HSP27 for treatment of female cancers** **Laila A. Jaragh-Alhadad,** *Kuwait University, Kuwait*
16:05-16:30	**Title: Association study of HIF-1α rs11549465 and VEGF rs3025039 genetic variants with diabetic retinopathy in Egyptian patients: Crosslinks with angiogenic, inflammatory, and anti-inflammatory markers** **Leqaa A. Moemen,** *Research Institute of Ophthalmology, Egypt*

E-Posters

	Title: A 4-year of HbA1C assay performance from Thailand in the European HbA1c Trial **Supaporn Suparak,** *Department of Medical Sciences, Ministry of Public Health, Thailand*
	Title: Resilience of glass fiber-modified advanced polymer composites **Catherine Vasnetsov,** *Caribbean Environment and Development Institute, Puerto Rico*

Networking & Refreshments 16:30-16:50

Closing Remarks

End of Conference

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KEYNOTE PRESENTATIONS

DAY 1

4th Edition of

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BIOGRAPHY

Dr. Landsberger is a Professor in the Nuclear and Radiation Engineering technical area. He has served on the faculty of the Cockrell School of Engineering since 1997. He has published more than 250 peer-reviewed papers and more than 200 conference proceedings mainly in nuclear analytical measurements and their applications in nuclear forensics, natural radioactivity and environmental monitoring of trace and heavy metals. In 2007, he received the Arthur Holly Compton award from the American Nuclear Society for outstanding achievements in education in nuclear science and engineering for designing and implementing one of the most advanced distance learning programs in the nation for nuclear engineers. In 2005 he received the Glenn Murphy Award from the Nuclear and Radiological Division of the American Society of Engineering Education, recognizing his notable professional contributions to the teaching of undergraduate and graduate nuclear engineering students.

S. Landsberger

Nuclear Engineering Teaching Lab, University of Texas at Austin, USA

Naturally occurring radioactive materials in oil exploration: How did this happen?

Perhaps the first scientific paper on the discovery of radioactivity in oil appeared in 1906 just a mere eight years after Becquerel discovered radiation emanating from uranium salts. The discovery of radioactivity captivated scientists and engineers for the following decades resulting in astonishing discoveries and many noble prizes. It was not until the 1980's that intense research in radioactivity in oil and gas exploration was re-kindled. In the last forty years, there has been a plethora of research conducted on radioactivity in oil and gas exploration with advanced nuclear analytical methods, leaching dynamics, and potential health effects. With more than 100 million barrels of crude oil being used on a daily basis, the long-term environmental impact is very significant. The goal of this paper is to give a historical overview of these topics and address future research.

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BIOGRAPHY

A/Prof Liza Forbes specializes in mineral flotation, with specific focus on flotation reagent chemistry, mineral surface chemistry and base-metal sulphide electrochemistry, with special attention to coarse particle flotation. Her main interest lies in integrating fundamental and applied aspects of flotation research, to develop new and improved processing technologies.

A/Prof Forbes currently leads the "Flotation Chemistry" group at the Julius Kruttschnitt Minerals Research Centre, Sustainable Minerals Institute, University of Queensland. She is also the Technical Director of the Collaborative Consortium for Coarse Particle Processing Research (CPR), as well as a UQ Node leader for the ARC Centre of Excellence for Eco-efficient Beneficiation of Minerals.

L. Forbes

Julius Kruttschnitt Mineral Research Centre, University of Queensland, Australia
ARC Centre of Excellence on Eco-Efficient Beneficiation of Minerals (CE200100009), University of Newcastle, Australia

Aerosol collector addition in coarse particle flotation

Mineral flotation is one of the primary separation stages in recovery of valuable minerals from ores. The flotation process requires the ore to be ground down to very fine sizes (<200 µm), a process that requires a tremendous amount of energy. It has been estimated that this energy accounts for 2 to 4% of global electricity consumption.

The ability to successfully perform flotation at coarser particle sizes has long been seen as the area where significant step-change improvements to energy efficiency of mineral processing operations could be made. Significant advances have made in the field of flotation equipment design, with the introduction of novel technologies such as fluidised bed flotation. However, no similar developments were made in the area of flotation chemistry.

Flotation makes use of chemical reagents known as collectors that selectively adsorb onto mineral surfaces rendering them hydrophobic. These minerals then attach to air bubbles and are "floated" out to the concentrate. An interesting new possibility is the use of aerosol collector addition, whereby collector reagents are introduced to a flotation system via the surfaces of bubbles rather than through the aqueous solution to the mineral particles. The concept of aerosol collector addition is not novel, but relatively poorly studied. The few studies that have focused on it have demonstrated that thermodynamically such methods result in a significant improvement in collector adsorption.

This work reviews the available literature on the underlying mechanisms of aerosol collector addition in flotation and how it impacts the collector coverage and resulting hydrophobicity of mineral particles. The review is performed in the context of the unique hydrodynamic environment of fluidised bed flotation of coarse particles. The goal of the work is to determine the potential of utilising aerosol collector addition to further boost the efficacy of coarse particle recovery.

BIOGRAPHY

I am a Physician Scientist in advanced heart failure and cardiac transplantation section at Massachusetts General Hospital and hold an appointment as an associate professor of Medicine at Harvard Medical School. My research has focused primarily on drug design and development using the three-dimensional structure of proteins. I have been involved in three major projects during my career. The first was direct renin inhibitors. Second was carvedilol. My most recent work has been designing growth factor mimetics for the TGF/BMP system. We have used the high-resolution three-dimensional structure of BMP 7, which we solved by x-ray diffraction techniques, as a starting point to develop BMP mimetics. We have designed over 30 compounds with slightly different effects that act through BMP signaling pathway.

William Carlson

Therapeutic by Design, Massachusetts General Hospital and Harvard Medical School, USA

Design of agonists for the selective activation of BMP signalling using the three-dimensional structure of BMP7 and a computer algorithm based on structure activity relationships and the physical chemical properties of amino acids

The BMP pathway is beginning to be appreciated for its clinical potential in countering the damaging effects of TGF in acute and chronic diseases, as well as cancer. Using the three-dimensional structure of BMP 7, which we solved by x-ray crystal crystallography, we were able to design small peptide analogs of BMP 7 that could activate the BMP pathway selectively. We developed an algorithm based on structure activity relationships that could predict the amino acid composition of the peptides and produce desired clinical effects. The process involves analyzing the surface accessible portions of the molecule and using a unique algorithm that incorporates desired properties and links these to the physical chemical properties of amino acids in the sequence. Using this algorithm, we have been able to design, synthesize and test an array of compounds. The prototype compound, THR123 has been shown to block apoptosis, inflammation, and fibrosis. In animal models of acute and chronic renal injury, THR123 was shown not only to protect against renal injury but also to reverse fibrosis and restore function. THR184 A congener of THR123 has progressed through phase 1 and phase 2 clinical trials. It has been shown to be safe and effective in treating acute kidney injury in patients undergoing cardiovascular surgery. In animal models of disease, THR123 and THR184 have been shown to be effective in preventing myocardial injury and also in killing prostate cells and breast cancer stem cells. They have also been shown to control endothelial mesenchymal transition, reversing this process in nonmalignant solid organ injury and cancer stem cells. The development of compounds that harness the power of the BMP pathway has great potential for the treatment of numerous debilitating diseases.

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DISTINGUISHED SPEAKER TALKS

DAY 1

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Automated SEM/EDS analysis for assessment of trace cross-contamination in 316L stainless steel powders for additive manufacturing

M.J. Balart[1], X. Hao[2] and **C.L. Davis[1]**

[1]University of Warwick, WMG - Advanced Manufacturing and Materials Centre (AMMC),UK

[2]Liberty Powder Metals, Materials Processing Institute, UK

316L is one of the most common grades of austenitic stainless steel and can be reliably additive manufactured. The rise of the powder metallurgy industry [1-7], particularly the metallic powder supply chain [8], has resulted in a significant increase in the complexity of alloys, products, and processing processes. This complexity is viewed as a source of risks, challenges and opportunities for the metal powder supply chain, powder processing and production technologies, and greater competitiveness [8]. The key challenges that could adversely affect the product's integrity are not only to prevent powder cross-contamination (CC), but also to mitigate solidification cracking.

This case study will showcase the use of automated SEM analysis for characterisation of contaminants in 316L powders for additive manufacturing applications. The presentation will also delve into examples of cross-contamination in powder materials reported in the literature, with consideration given to contaminant type, size and form in the powder (discrete particle or embedded in powder) and the chemical analysis method to detect the contaminant. Three additive manufactured 316L samples were built using selective laser melting (SLM) from three different types of 316L stainless steel powders (< 150 µm) produced by air-melted gas atomization (AMGA) from two suppliers. Two (from the same supplier) out of the three AM 316L samples cracked, in which cases welding diagrams could not normally account for. EBSD phase maps in all three AM samples exhibited a fully austenitic microstructure across the whole sample. Microcracked regions in AM samples were found to have local enrichment of Ni, Cu and P. Automated SEM/EDS analysis on feedstock powder samples produced for cross-section inspection revealed a fine, foreign particulate contaminant entirely embedded in a 316L powder particle, thought to come from NiCrCuP alloy cross-contamination during atomization. This sort of contamination would not have been found by examining powder mounted onto a SEM stub, a usual method for assessing powder quality. Based on this investigation, it is suggested that any standardized methodology for powder quality control include automated SEM/EDS analysis on powder cross-sections to maximise the possibilities of detecting and identifying fine cross-contaminants embedded within the powder.

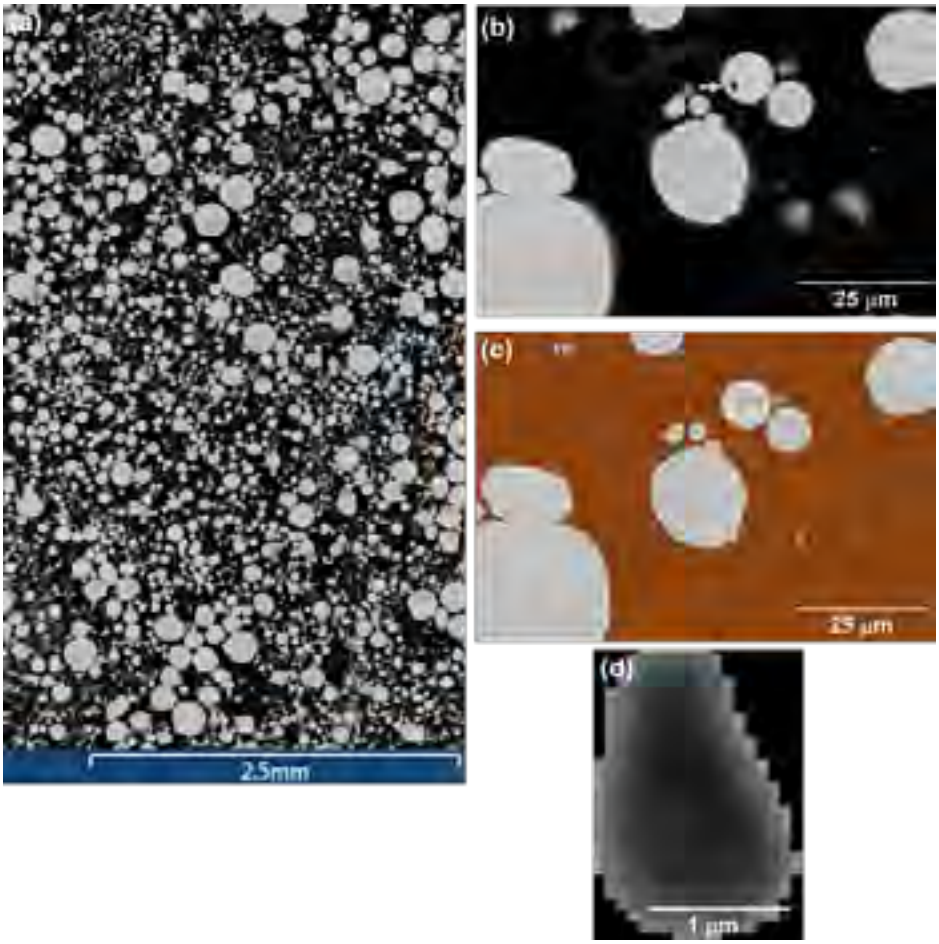

Figure: *BSE macrograph for the 316L < 150 µm powder B1 showing the area of analysis: 59 x 85.8 x 10-6 mm2 size of field, 6043 number of fields, 16.2 mm2 area of resin and 14.4 mm2 area scanned. A fine, foreign particulate contaminant (arrowed) completely embedded in a 316L powder particle (b) BSEI, (c) Imaging from a single grey threshold for detecting the contaminant and (d) BSEI of particulate contaminant in (b) [9].*

Table: *EDS analysis (wt pct) from the NiCrCuP alloy particulate contaminant in the Figure*

Ni	C	Cr	Cu	O	Si	P	Fe
52.6 ± 1.1	11.2 ± 1.5	10.0 ± 0.3	7.2 ± 0.5	5.7 ± 0.6	5.7 ± 0.2	4.5 ± 0.3	3.0 ± 0.2

Biography

María Balart received her bachelor's degree at the University of Barcelona in chemistry in 1994, her PhD at the University of Birmingham in 2000 for her work on structure-property relationships in microalloyed steels. She has maintained a research interest in this area. She conducted her postdoctoral research at the Open University, the University of Birmingham, Brunel University London and Warwick University. Currently, she is a project engineer at the Energy Innovation Centre (EIC) in the Warwick Manufacturing Group (WMG) working on projects related to battery forensic characterization.

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A decreased response to resistin in mononuclear leukocytes contributes to oxidative stress in nonalcoholic fatty liver disease

Plácida Baz[1], Cecilia C Garcia[1], Bárbara Piotrkowski[2,3], Daniel Poncino[4], Javier Benavides[5], Luis Colombato[5], María Laura Reyes Toso[6,7], Silvina Yantorno[6,7], Valeria Descalzi[6,7], Gabriel E Gondolesi[6,7], Cesar G Fraga[2,3] and **Alejandra C Cherñavsky[8]**

[1]Facultad de Farmacia Y Bioquímica, Instituto de Inmunología, Genética Y Metabolismo (INIGEM), CONICET-Universidad de Buenos Aires, Hospital de Clínicas José de San Martín, Argentina
[2]Facultad de Farmacia Y Bioquímica, Universidad de Buenos Aires, Argentina
[3]Instituto de Bioquímica Y Medicina Molecular (IBIMOL), Universidad de Buenos Aires-CONICET, Argentina
[4]Sección Hepatología, Servicio de Gastroenterología, Sanatorio Dr. Julio Méndez, Argentina
[5]Sección Hepatología, Servicio de Gastroenterología, Hospital Británico de Buenos Aires, Argentina.
[6]Unidad de Hepatología, Cirugía Hepatobiliar Y Trasplante Hepático, Hospital Universitario Fundación Favaloro, Argentina
[7]Instituto de Medicina Traslacional, Trasplante Y Bioingeniería, Universidad Fundación Favaloro, Argentina
[8]Facultad de Farmacia Y Bioquímica, Instituto de Inmunología, Genética Y Metabolismo (INIGEM), CONICET-Universidad de Buenos Aires, Hospital de Clínicas José de San Martín, Argentina

Deregulation of immune response and oxidative stress contribute to nonalcoholic fatty liver disease (NAFLD) Resistin is a physiological modulator of inflammation and redox homeostasis of different cell types. Increased resistin serum concentration and the direct association between resistin hepatic expression and NAFLD severity suggest thatresistin participates in NAFLD pathogenesis. To evaluate resistin-induced regulation of redox homeostasis in mononuclear leukocytes from NAFLD patients and controls.

Methods: We evaluated basal and resistin-mediated modulation of reactive oxygen species (ROS) and glutathione contentby flow cytometry, and antioxidant enzyme activities by spectrophotometry.

Results: Peripheral blood mononuclear cells (PBMC) from NAFLD patients showed higher ROS content and glutathione peroxidase activity and lower glutathione content, superoxide dismutase and glutathione reductase activities than control PBMC. Resistin decreased ROS levels and superoxide dismutase activity and increased glutathione reductase and catalase activities in PBMC from controls but not from patients. Resistin decreased glutathione content in PBMC from control and NAFLD patients, with greater effect on patient cells. Basal and resistin-modulated ROS levels were directly associated with obesity-related risk factors for NAFLD. Hepatic myeloid cells and T-lymphocytes from NAFLD patients showed higher basal ROS content than cells from controls. Resistin decreased ROS levels in hepatic T-lymphocytes from controls but not from patients.

Conclusions: Resistin regulates redox homeostasis in mononuclear leukocytes. A decreased response to resistin in leukocytes from NAFLD patients is associated with an impaired redox homeostasis.

Biography

Pharmacist and Biochemist, graduated from the University of Buenos Aires, specialist in Hematology and Immunology. Principal professional at the Flow Cytometry and cell Sorting core Facility of the Immunogenetics Laboratory; Institute of Immunology, Genetics and Metabolism (INIGEM), Clinical Hospital José de San Martín, University of Buenos Aires (UBA), National Council for Scientific and Technological Research (CONICET), Buenos Aires, Argentina. Professor of different postgraduate levels at the University of Buenos Aires. Member of the River Plate Group of Flow Cytometry. Long experience in Clinical Analysis Diagnosis and Research.

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Subtle early-warning indicators of landfill subsurface thermal events

Andy Davis, C. Whitehead and **M. Lengke**
Geomega Inc, USA

It is generally accepted that landfills undergo at least four phases of decomposition, 1) an initial aerobic phase, 2) an anaerobic acid phase, 3) an initial methanogenic phase, and 4) a stable methanogenic phase. While landfill fires are common, recently anoxic subsurface heating events (ASHEs) have been recognized, potentially catalyzed by aluminum waste. This paper reviews two such events to forensically examine if there are predictable early warning signs in the gas record prior to the onset of an ASHE that could facilitate early action.

At the Countywide Recycling and Disposal Facility in East Sparta, Ohio, decreasing methane (CH_4) in landfill gas was identified in a post-mortem analysis as an early indicator parameter (IP) of an abnormal landfill condition because the ASHE inhibited methane-producing microorganisms. Here the CH_4:CO_2 ratios also decreased to < 0.8 at least one year prior to onset of the full-fledged ASHE in some gas wells.

Landfill A was a municipal solid waste landfill that operated through December 2004. The landfill gas and temperature profiles appeared normal after closure until 2009, when landfill gas characteristics in several wells started to evolve towards an upset condition, with decreasing methane (CH_4 <43%), increasing carbon monoxide (CO > 500 ppm), increasing balance gas (>20%) and a CH_4/CO_2 ratio decreasing below 0.8.

The evolution in sequencing of ASHE IPs was, 1) declining CH_4, followed by, 2) increasing CO_2 and % balance gas and, then 3) CO before onset of the ASHE. Subsequently, 4) leachate volumes increased as did, 5) the BOD/COD ratios and benzene in leachate, and finally 6) release of landfill contaminants to groundwater. These multiple lines of evidence suggest that operators should carefully evaluate data trends as indicators of potential upset conditions. The gas profiles in many Landfill A gas wells were similar to those at Countywide and appear to be predictable by a Landfill Fire Index (LFI) based on temperature, CO_2 and CH_4 patterns. While there were sporadic exceedances of the NSPS temperature (131°F), and above the Higher Operating Value (140°F) in some wells, the change in landfill gas IP signature and the LFI appears to have pre-dated the major thermal event by between ½-3 years, depending on the well.

Biography

Dr. Davis has solved environmental problems for industrial clients for over 25 years, primarily at RCRA and CERCLA sites. As an Adjunct Professor at the Department of Geological Sciences at the University of Colorado, Dr. Davis taught *The Fate and Transport of Organic Compounds in the Environment*. He has been the Principal Investigator (PI) for >20 NEPA-related mining projects, many in north-east Nevada and has routinely interacted with NDEP, NDWR, the US EPA and BLM. He has managed projects at environmental sites in the US and abroad, 30 in California. Dr. Davis has played soccer for >60 years and coached kids soccer and basketball for 18 years.

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Total mandible and bilateral TMJ reconstruction combining a customized jaw implant with a free fibular flap

B.A. Pesucci[1], F.A. Govoni[1], R. Pistilli[1], V.A. Marcelli[1], I. Aboh[1], C. Macro[1], R. Pucci[1], N. Felici[2] and **M. Ornelli[2]**

[1]Maxillo Facial Surgery Unit, San Camillo Forlanini Hospital, Italy
[2]Plastic and Reconstructive Surgery Unit, San Camillo-Forlanini Hospital, Italy

The need for whole mandibular bone reconstruction and bilateral joint replacement is fortunately rare, but it is an extremely challenging topic in maxillofacial surgery, due to its functional implications. CAD-CAM tech-niques development has opened new broad horizons in the surgical planning of complex maxillofacial reconstruc-tions, in terms of accuracy, predictability, and functional cosmetic results. The review of the literature has revealed a small number of scientific reports on total mandibulectomy including the condyles, with only eleven cases from 1980. Most of the works describe reconstructions secondary to dysplastic or inflammatory diseases affecting the lower jaw. The aim of this work, reporting a rare case of massive fibrous dysplasia of the whole mandible, is to share our experi-ence in the management of extended mandibular and bilateral joint reconstruction, using porous titanium patient-specific implants.

The authors present a 20-year-old male patient suffering from massive bone fibrous dysplasia of the mandible. The mandibular body and both the rami and the condylar processes had been involved, causing severe functional impairment, tooth loss, and facial deformation. The young patient, after repeated ineffective conservative surgical treatments, has required a biarticular mandibular replacement. Using virtual surgical planning (VSP) software, the authors, in collaboration with medical engineers, have created a custom-made original titanium porous mandibular implant, suspended from a bilateral artificial temporomandibular joint. The mandibular titanium implant body has been specifically designed to support soft tissues and to fix, in the alveolar region, a free fibular bone graft, for delayed dental implant prosthetic rehabilitation

Conclusion: The surgical and technical details, as well as the new trends in mandibular reconstructions using porous titanium implants, are reported, and discussed, reviewing literature reports on this topic. Satisfactory functional and cosmetic restorative results have been obtained, and no major complications have occurred. The patient, currently in the 18th month clinical and radiological follow-up, has recently completed the functional restoration program by an implant-supported full-arch dental prosthesis.

Biography

Prof. Dr. Bruno Andrea Pesucci Born in Milan 14/11/1954 Specialization in Maxillo Facial Surgery Specialization in Odontostomatology Director of Maxillo Facial Surgery Unit - S.Camillo Forlanini Hospital - Rome Past President of the Maxillo Facial Surgery Society Teacher at the Course of Specialization in Maxillo Facial Surgery at the University La Sapienza - Rome Teacher at the Course of Anterior Skull Base Surgery and Anatomic Dissection - Palm Beach (Florida) Teacher at the Course of Specialization in OSAS Syndrome Since 1996 Director of Maxillo Facial Surgery in the Oncologic Multidisciplinary Group of San Camillo Hospital.

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Combination of Betulinic acid fragments and Carbonicanhydrase inhibitors – A new drug targeting approach

R. Paschke and **A. Funtan**

Martin Luther University Halle-Wittenberg, Germany

Carboanhydrase IX (CA IX), which is highly overexpressed in hypoxic tumors, offers the possibility of targeted treatment of various cancers such as breast carcinoma [1-3]. Carboanhydrase inhibitors are well studied and already in clinical applications, whereas relatively little is known in the area of drug conjugates for carboanhydrases. The aim of this work was to develop drug conjugates based on a combination of CA IX inhibitors with cytotoxic and natural product betulin/betulinic acid (BE/BA) [4-6], which are able to bind specifically to CA IX, accumulate in the tumor tissue and exert their cytotoxic effect there. A number of drug conjugates were synthesized and their binding affinity for CA IX was determined by an enzymatic esterase assay. All conjugates and their precursors were tested for cytotoxicity by sulforhodamine B (SRB) assay.

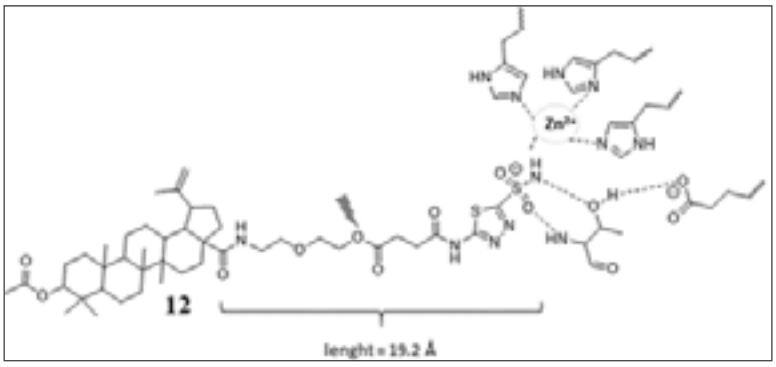

Figure. *Bifunctional conjugate of betulinic acid, a semi-labile linker and acetazolamide.*

Biography

Place of work:

BioCenter of the Martin-Luther-University Halle-Wittenberg, Weinbergweg 22, 06120 Halle (Saale), Germany

Education:

Studies in Chemistry, Martin-Luther-University Halle-Wittenberg

Diploma („magna cum laude")

Dissertation („magna cum laude ") „Synthesis of new 2,6,7-Trioxa-bicyclo(2.2.2)octane- und 5-n-Butyl-pyridine-2-carbonic acid derivatives with liquid crystalline properties"

Habilitation:

Metal complexes as functional units for the formation of structures with liquid crystalline or cytotoxic properties

Academic and Research Career:

Research Assistant, Chemical Institute, Martin-Luther-University Halle-Wittenberg

Post Doc Research, University of Southampton, University of Hull

Senior Researcher, Chemical Institute, Martin-Luther-University Halle-Wittenberg

Head of the BioCenter of the Martin-Luther-University and Head of the Medicinal-Pharmaceutical Chemistry unit.

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Consideration of net-zero concrete toward a carbon recycling society by a mineral carbonation using alkali wastes

Y. Izumi[1], A. Iizuka[2] and **H.-J. Ho[2]**

[1]Sustainable Development Innovations (SDIs), Japan

[2]Center for Mineral Processing and Metallurgy, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Japan

Concrete is composed of 70-80wt% of fine and coarse aggregates and the rest of hydrated cement. Since a carbon footprint of the concrete is mainly CO2 emissions during cement production, use of low carbon cement is a key element in developing net-zero concrete. Approximately one-third of the total CO_2 emissions from cement production resulting from the fuel combustion can be reduced by using energy conservation, fuel conversion and innovative technologies such as CCU&S. However, substantial process-related CO_2 emissions from limestone decarbonation during calcination process are almost unavoidable, and effective countermeasures are required to achieve net-zero emissions.

The authors recently developed a mineral carbon capture and utilization (MCC&U) that is one mineral carbonation technology where CO_2 is chemically sequestered using calcium in alkali industrial wastes such as concrete sludge and demolished concrete to form recarbonates (i.e., $CaCO_3$). MCC&U is a carbon recycling system and the recarbonates are utilized for several applications shown in Figure.

In this presentation, in addition to the use of low carbon cement, a part of fine aggregates is replaced by recarbonates using concrete sludges generated at the ready mixed concrete plant and CO_2 gas to be generally stored stably in concrete under normal conditions. A carbon dioxide containing concrete (CDC)

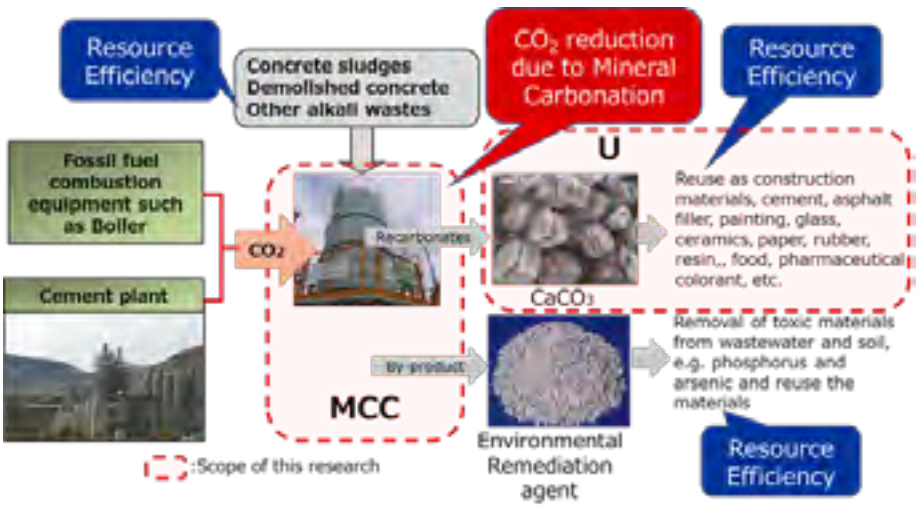

Figure: *Outline of MCC&U Technology*

is mixed under 460Kg/m^3 of cement intensity and 37% of water/cement ratio using a 25 litter-concrete mixer. Table shows there is no difference of properties between reference and CDCs without loss of strength, where $CaCO_3$ contained in CDC-1 and CDC-2 are 0.7wt% and 1.4wt% of cement, respectively.

The carbon footprints are calculated using newly proposed GHG accounting methodology of MCC&U in the cement industry. To achieve net-zero concrete while maintaining concrete quality, further study on approximately 60 times addition of $CaCO_3$ reused for CDC-1 would be required.

Testing items (unit)		Specification	Reference	CDC-1	CDC-2
Slump (cm)		18±2.5	20.0	18.0	19.0
Air content (%)		4.5±1.5	5.2	4.3	5.9
Temperature (℃)		10 - 30	17	17	17
Chloride content (kg/m^3)		below 0.30	0.044	0.047	0.046
Compressive strength (N/m^2)	7 days	~42×0.7	48.9	52.3	49.2
		(Ratio)	-	**106.9%**	**100.6%**
	4 weeks	42×0.85	61.1	61.5	59.4
		(Ratio)	-	**100.7%**	**97.2%**

Table: *Comparison of CDC concrete's properties with reference concrete*

Biography

He joined Onoda Cement Co. Ltd. (then Taiheiyo Cement Corporation) in 1978 following post-doctorate research at the University of Illinois, USA. He had been responsible for participating in the Cement Sustainability Initiative of WBCSD (then Global Cement and Concrete Association) since 2000. He contributed to the IPCC WG III on the Assessment Report (2007, 2014 and 2021) as an expert reviewer and the IEA program on a development of cement technology roadmap (2009).

In 2010, he transferred to Japan Cement Association and externally served to Research Institute of Innovative Technology for the Earth as the Climate Technology Center & Network project manager under UNFCCC on low carbon technologies including an MCC&U technology during 2017 and recently founded SDIs to support an implementation of the technology globally.

He holds a Ph.D. in Material Science and Engineering from Northwestern University, Evanston Illinois, USA.

Tailor-made alkaliphilic and thermostable fungal laccases for industrial wood processing

Michael Lecourt
FCBA Institut Technologique, France

Wood is a biomaterial used for several applications. Some are evident, such as furniture or buildings. Some are possible thanks to chemical extractions, making it possible to obtain and valorise chemical derivatives. They are cellulose, hemicelluloses or lignins, for instance obtained during kraft pulp production or biofuel processings. Focus was paid on lignin valorized as novolaque adhesives used for ply bonding in plywood or fibres in fiberboard. Original treatments were applied for modifying reactivity of lignin substituting phenol by 80% but also halving formaldehyde content. Additionally to sourcing, considering various species and processes, alkaliphilic fungal laccases assisted modification of lignin made it possible to vary lignin reactivity. This was measured on resins by viscosity after precondensation and solidification time. Tested on plywood and MDF productions, lignin played the role of coreticulant with phenol and formaldehyde in resin synthesis and contributed to lowering environmental impact of products keeping performances as high as requested.

Biography

Michael Lecourt works for 20 years on research and development projects related to wood valorisation. Based in Grenoble (France), he is a FCBA collaborator. Starting on wood quality related to products, he developed skills on enzymatic treatment applied onto natural fibres, but mainly wood, prior to mechanical treatments. Some of these researches are now commonly applied during processing. Focus is now paid on wood based boards for improving performances, reducing harmful chemical uses and lowering environmental footprint of products.

Carbon dioxide (CO_2) utilization through chemical and electrochemical conversion

Geoff Wang[1], Ping Chen[1], Muxina Konarova[1] and **Aaron Li[2]**

[1]School of Chemical Engineering, The University of Queensland, Australia

[2]School of Chemical Engineering, The University of Melbourne, Australia

Carbon dioxide (CO_2) utilization holds promise to alleviate negative climate impacts from anthropogenic CO_2 emissions in an economically feasible way. This talk presents research and development studies on CO_2 utilization through chemical[1]) and electrochemical[2~4]) conversion, which aims to develop sustainable technology, especially for iron and steel industries5). Through chemical and electrochemical conversion technologies, CO_2 can be converted into valuable chemicals such as ethanol, formic acid and/or CO by using green power (such as from hydro, solar and wind energy, even the low-grade waster heat). The proposed chemical and electrochemical conversions of CO_2 may stand out because of its mild operation conditions, ease of process control, modular design that is easy for scale-up, and flexibility to retrofit with existing carbon-intensive industrial infrastructures such as steel mills based on ironmaking blast furnace route. At present, however, challenges still remain impeding its practical application. These challenges include sluggish reaction rate, poor selectivity, long-term stability, and integration with specific industrial processes, all contributing to an insufficient energy efficiency and a high cost for upstream CO_2 capture and downstream product separation. Herein, it is worthy attempting to circumvent these challenges by optimizing its local catalytic environment (i.e., electrode/electrolyte interfaces)[2,3]) and investigating gas/liquid/electron multi-flow phenomena[4]). By tailoring the property of the either electrode catalyst or the electrolyte, we could significantly improve the selectivity of the CO_2 conversion and reduce the complexity of the carbon capture and utilization processes. In addition, the developed technologies can be potentially applied or further developed for other clean energy processes such as the hydrogen production.

Biography

Professor Geoff Wang received his PhD in Chemical and Metallurgical Engineering from the Northeastern University, Shenyang, China in 1990, and then worked in Wuhan University of Science and Technology in China for 5 years and about 2 years at University of New South Wales, Australia. He joined the University of Queensland in 1996 unit now. His research activity and interests are directed towards developing energy and environmental technologies dealing with the coal and steel industries. He has been active and performed many research programs in clean energy and low-carbon technologies such as pulverized coal injection into blast furnaces, hydrogen production through lower emission coal combustion, and chemical and electrochemical conversion of CO_2 to fuel or reusable chemicals.

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Water and its dielectric signature: New marker for biosensing

Yuri Feldman

Department of Applied Physics, The Hebrew University of Jerusalem, Edmond J. Safra Campus, Israel

Whenever water molecules interact with either dipolar or charged systems, the main water dielectric relaxation peak broadens. If a solute is dipolar in nature, new solute-water clusters are created due to dipole-dipole interactions. It leads to the "red shift" of the dielectric loss maximum frequency. In the case of ionic solutions, another cluster structure develops, due to dipole-charge interactions and a "blue shift "is observed. In the general case when a solute molecule has both charged and dipole groups, the dielectric loss maximum demonstrates a "red" or "blue" shift, depending on the entity concentration. In all aqueous solutions, the water-solute interactions can be considered as dipole-matrix interactions in which water is the dipole subsystem. The phenomenological 3D trajectories approach was applied to the results of isothermal dielectric measurements of different concentrations of the following aqueous solutions: Hydrocarbons, NaCl and KCl, AMP and ATP, Amino Acids and proteins [1-5]. The parameters of the main water peak define a trajectory that can clarify the nature and rate, at which water interacts with the solute. In this paper, we extend this approach from comparatively simple solutions to the complexity of Red Blood Cells (RBC) suspensions by monitoring the RBC cytoplasm under different external conditions [6,7]. Dielectric measurements of RBC suspensions in the frequency region of 100 MHz to 50 GHz as a function of aging or external glucose concentration also reveal a distinct time point or glucose concentration after which the spectra are radically changed. The conclusion is that the dielectric response of the cytoplasm in microwaves is due to the water therein and its interaction with physiological active components in cytoplasm. This opens a window of opportunity to exploit this for the non-invasive monitoring of diabetes or to non-invasive control of the quality of Stored RBC in a Blood bank in order to manage the inventory.

Biography

Yuri Feldman received the M.S. degree in radio physics and Ph.D. degree in molecular physics from the Kazan State University, Kazan, USSR, in 1973 and 1981, respectively. From 1973 to 1991, he was with the Laboratory of Molecular Biophysics, Kazan Institute of Biology, Academy of Science of the USSR. In 1991, he moved to The Hebrew University of Jerusalem, Israel, where he is currently a Full Professor and the Head of the Soft Condensed Matter Physics Laboratory. He has spent over 40 years in the field and has more than 400 scientific publications related to dielectric spectroscopy and its applications. He holds 15 patents in the areas of electromagnetic properties of the matter. In 1992 and 2010, the Israel Government acknowledged his work with an award for the outstanding contribution to the development of Israel Science; in 1998, he received the Kaye Award for the best innovation and invention. Feldman is a Director of the Centre for Electromagnetic Research and Characterization (CERC); he is a Member of the Boards of International Dielectric Society (IDS) and International Society for Electromagnetic Aquametry (ISEMA). His current interests include broadband dielectric spectroscopy in frequency and time domain; theory of dielectric polarization and relaxation; relaxation phenomena and strange kinetics in disordered materials; electromagnetic properties of biological systems *in vitro* and *in vivo.*

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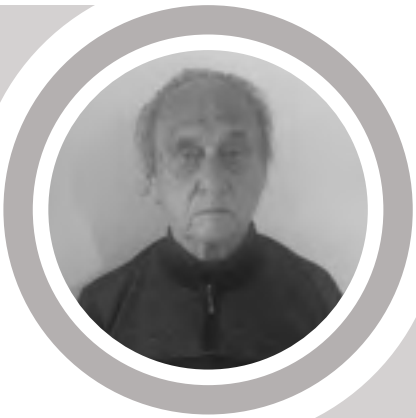
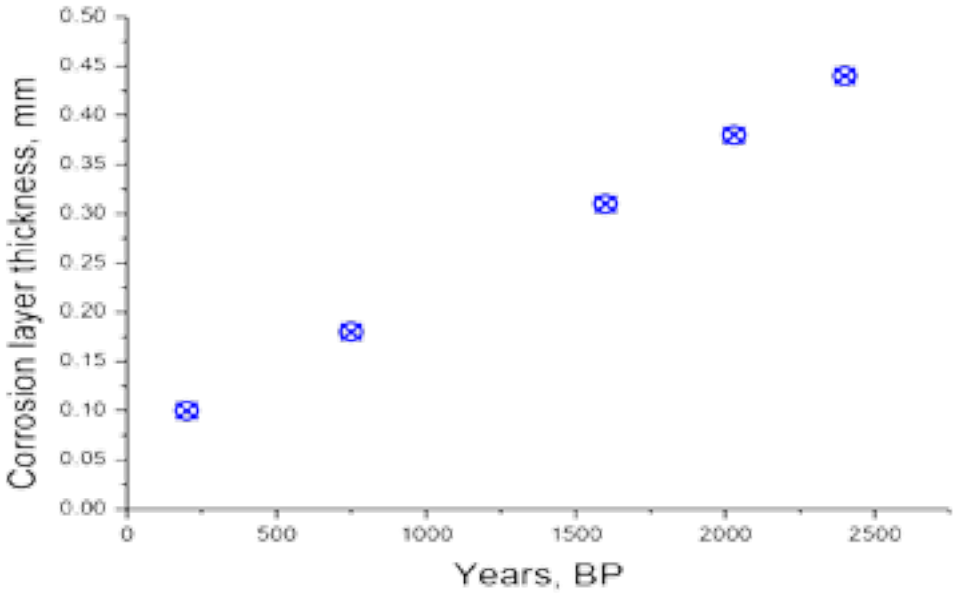


Direct optical measurement of corrosion layer thickness of archaeological lead artifacts; A new simpler dating method

S. Shilstein, J. Kettering, Y. Sharvit and **S. Shalev**

[1]*Weizmann Institute of Science, Israel*
[2]*Haifa University, Israel*
[3]*Antiquity Authority, Israel*
[4]*Haifa University, Israel*

A method for dating lead archaeological objects based on measuring the thickness of the layer of corrosion products by optical examination of their cross-sections with a relatively low magnification is proposed. In comparison with already existing methods for dating lead such as electrochemical and magnetometric methods, the optical method is simpler to use and accurate at least as the previous methods and can be used lead in the field.



Dependence of corrosion layer thickness upon time before present.

Chemical profile of tropical red wines from the Submiddle São Francisco Valley, Brazil

Carlos Artur Alves

Centro Universitario Inta - Uninta, Brazil

São Francisco Submiddle Valley (SFSV) is the pioneer wine-producing region in tropical countries, having the first structured and filed Geographical Indication request regarding these conditions. Also, SFSV is the principal Brazilian table grape producing-region and an important producer of sparkling and red wines. Then, red wines have great growth potential in SFSV, since red grapes are the main adapted to the geographical conditions, and these wines having wide scope for market growth. Further, this major adaptation and the red wines market share may be related to phenolics, which play an important role in sensorial traits and aging ability. Phenolic compounds have been related to antioxidant activity, mainly some of catechins, anthocyanins, and phenolic acids. The paper "Chemical typicity of tropical Tannat red wines from Sub-Middle São Francisco Valley, Brazil" discuss the phenolics compounds and antioxidant activity in Tannat and Syrah wines from the Brazilian Northeast, which may bring important discussions concerning how the terroir may to maximize the phenolics production pathways. Furthermore, all discussion about the region may touch the global warming, and how the tropical regions may be a laboratory to temperate regions in the future.

Biography

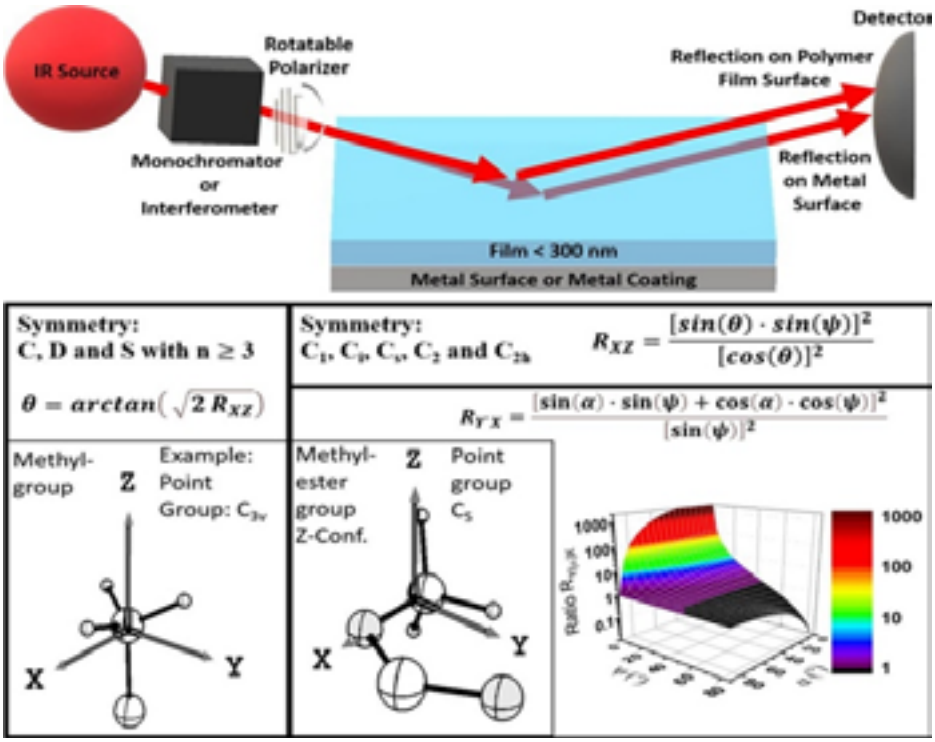
Carlos Artur N. Alves is a food science and gastronomy professor at the UNINTA University Center, Brazil, with expertise in wine, wine chemistry and sensory analysis. His research in the Master degree focuses in phenolic compounds and deterioration study of red wines from the tropical region São Francisco Sub-middle Valley, in Brazil Northeast. Professor Artur Alves has received a honor bachelor's degree from the Federal University of Ceará. He has published research papers in international journals, as the International Journal of Gastronomy and Food Science, and the Journal of Food Science and Techonology. He is Sommelier student at the Sommelier Brazilian Association (ABS) and Association de la Sommellerie Internationale (ASI).

Orientation analysis of polymer thin films on metal surfaces via IR absorbance of the relative transition dipole moments

Andreas Früh[2], Sven Rutkowski[2], Igor O. Akimchenko[2], Sergei I. Tverdokhlebov[2] and **Johannes Frueh[1]**

[1]Faculty of Medicine and Health, Ministry of Education, Harbin Institute of Technology, PR China
[2]National Research Tomsk Polytechnic University, Russian Federation

Modern technology has increasing requirements for thin film based electronic devices. Many surface and electronic properties strongly depend on the orientation of the material. Industrial development has a need for cheap, non-destructive, and fast orientation analysis in different conditions. Infrared-orientation analysis is less represented in literature compared to other orientation methods, while offering a lot of unique advantages. In this respect for thin polymeric films, we propose infrared (IR) absorbance-spectroscopy near metal surfaces to distinguish the orientation of different molecular segments. By use of the ratio method, the calculation of the orientation becomes mostly independent from the angle of incidence and averages out aperture errors



of the measurement setup, hence the given solutions are generally applicable for many setups. For the most common point groups, the hereby-presented mathematical solution is valid for thin films cast on metal surfaces. Extensive quantum mechanical calculations of the transition dipole moments are avoided for known IR spectroscopy bands. The detailed application of the given IR orientation analysis is demonstrated for the polymers polystyrene, polyethylene glycol, poly(methyl methacrylate) and polyvinyl acetate. Each segment of these polymers is analyzed for the preferred molecular orientation in respect to the surface as exemplary shown in figure below.

Biography

Studies and PhD in Tübingen University with focus on physical chemistry. Topic of PhD thesis is stability and orientation of advanced semi-conduction polymer materials. Orientation of semi-conductive polymers have great influence on the absorption and conductive behavior. Existing methods of orientation analysis were often either expensive or do not cover all segments of polymeric material. By use of IRRA-spectroscopy insight on the orientation of thin polymer films is extracted. By this means I specialized in FTIR-, Fluorescence, UV-Vis and Raman spectroscopy for extensive research on polymeric material. Post-doctoral research in international projects with topics in spectroscopic analysis methods are ongoing. Current projects include development and enhancement of imaging microscopy for use in medical technology as contamination control.

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KEYNOTE PRESENTATIONS

DAY 2

4th Edition of

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BIOGRAPHY

My degrees include a BS-Chemical Engineering, an MS-Mineral Processing, and a DSc-Extractive Metallurgy.

I am President of T. P. McNulty and Associates, Inc., a global consulting firm helping mineral industry clients evaluate, develop, and/or adopt new technologies for improved resource recovery, reduced costs, and minimum environmental impact. I have provided consulting services in processing of the ores of copper, silver, gold, uranium, Rare Earth Elements, and many nonmetallic minerals.

Earlier responsibilities included President of Hazen Research, Inc., a process development contractor, and VP-Technical Operations for Kerr-McGee Chemical Corporation. Initially, I worked for The Anaconda Co. in various operating management and technical roles, including Corporate Director-R&D.

My memberships include various professional societies and I was elected in 2004 to the National Academy of Engineering. I have been granted patents and published over 40 papers on various aspects of mineral processing and related topics.

Terry McNulty

T.P. McNulty and Associates, Inc., USA

Processing the ores of rare earth elements

The Rare Earth Elements (REE) are 15 elements in the atomic number range 57 through 71. Since the lowest member of the series is lanthanum, the REE are referred to as "lanthanoids", and they occupy the f block in the Periodic Table. The "light" elements (LREE) include lanthanum through gadolinium, while the heavier HREE comprise terbium through lutetium. In the LREE, the number of unpaired 4*f* electrons increases as electrons are added to the 4f levels, whereas a decrease in unpaired electrons occurs as electrons are added to the 4*f* levels in the HREE. In all cases, the progressively added electrons are distant from the valence electrons. The practical consequence of this behavior is that all of the REE exhibit very similar chemical behavior, especially in aqueous solutions.

REE ores usually contain no more than several weight percent REE, and there are hundreds of examples among the world's known mineral deposits that vary geologically from hard-rock pegmatites to marine sediments to several types of clays. With the exception of some salt-like aqueous resources in China, economic viability requires that the desired minerals be concentrated by upgrading methods ranging from those taking advantage of differences in specific gravity or magnetic or electrostatic response to selective flotation that relies on surface physical chemistry in an aqueous suspension of pulverized ore fragments. The concentrate, typically containing multiple REEs, must then be treated chemically to separate and then to purify individual elements as oxides or carbonates.

Early isolation and purification techniques, including nitrate crystallizations that typically required 15,000 repetitions, were replaced by resin ion exchange, followed by chromatographic elution. Increased demand and competition finally resulted in liquid-liquid extraction ("solvent extraction", or "SX"). SX remains the preferred route, but it is imperfect

and usually requires about 1,500 stages of mixer/settlers for the organic and aqueous phases.

During the last five years, there has been explosive growth in geological exploration and R&D directed toward discovery, resource development, and treatment of mineral assemblages that often are very low-quality and unresponsive to conventional processing. The REE industry is at the intersection of conflicting pressures. There is universal public support for "green" energy and sustainability; however, mining and processing of REE deposits have an abysmal record of disdain for human health and environmental needs and are incompatible with our demands for a clean, socially responsible, and reliable supply chain.

Chemists and extractive metallurgists face formidable challenges, but great opportunities, in the rapidly accelerating demand for these unusual elements that are essential to the manufacture of wind turbines, electric vehicles, medical devices, and many other applications vital to our evolving needs.

This presentation will describe current upgrading, separating, and refining technologies and will discuss potential ways of improving REE production efficiencies while reducing costs, thereby ensuring affordability of the end uses.

BIOGRAPHY

Franz-Josef Meyer-Almes is Professor of Biochemistry at the University of Applied Sciences Darmstadt in Germany. He earned his Diploma in Chemistry at the Georg-August-University of Göttingen (Germany) in 1991 and his PhD in Biophysical Chemistry from the same University in Göttingen. The main focus of his research is in thermodynamics and kinetics of protein-ligand and protein-protein interaction, reaction kinetics and mechanism, biological assay development, drug design, medium throughput screening, fluorescence spectroscopy and design of experiment. These methods are used to develop novel active substances against human histone deacetylases, which are validated targets in oncology, but also other neurodegenerative and age related diseases.

F.-J. Meyer-Almes

Darmstadt University of Applied Sciences, Germany

HDAC inhibitors with non-hydroxamate warhead

Compounds with a thiazolidinedione (TZD) functionality, so called glitazones, are known as PPARγ-activators and anti-diabetic drugs. The mode of action of these glitazones has extensively be investigated and is known in great structural details. PPARγ is a prominent target with a key role in the regulation of glucose homeostasis and lipid metabolism. However, PPARγ is also vital to cancer cell growth regulation. Moreover, a combination treatment with histone deacetylase (HDAC) inhibitors and PPARγ agonists increased cytotoxic effects against various cancer cell lines in a synergistic manner resulting in proliferation arrest and apoptosis. A closer view at the TZD group led us to conclude that TZD compounds should be in principle capable of binding to the catalytic zinc ion at the bottom of the active site of zinc dependent members of the HDAC protein family. This hypothesis has been confirmed by molecular docking. Therefore, we investigated the inhibitory effect of 225 TZD-analogs on HDAC4 and HDAC8. Different clusters with dual acitivity against PPARγ and HDAC4, or VEGFR-2 and HDAC4 were identified and mechanistically analyzed. Most potent compounds exhibit pronounced antiproliferative effects against tumor cells, and are also able to induce in vivo tumor regression in animal xenograft tumor models.

BIOGRAPHY

Dr. Dimitrios Kotzias (Ph.D in chemistry, University of Bonn/ Germany was Acting Director of the Institute for Health and Consumer Protection (IHCP) and Head (retired) of the Chemical Assessment and Testing Unit at the European Commission's Joint Research Centre (JRC), Ispra/ Italy. His research activities focused on trace analysis of organic compounds in complex matrices, photochemical and photocatalytic reactions, photochemical oxidants, indoor air quality and exposure assessment to chemicals and chemical mixtures. Founding member and for many years President of the Mediterranean Scientific Association of Environmental Protection (MESAEP). Dr. Kotzias has coordinated/participated of/in several EU funded research projects. He is author or co-author of ca. 250 reports and papers published in peer reviewed scientific journals.

Dimitrios Kotzias

Form. Sen. Official of the European commission's Joint Research Centre, Head of Unit Chemical Assessment and Testing, Institute for Health and Consumer Protection, Italy

Application of heterogeneous photocatalytic technology for the degradation of gaseous priority pollutants in ambient air and indoor environments

In the last decades, numerous studies indicated the substantial role semiconductors play in photocatalytic processes for environmental applications. In the present work, the focus is on TiO_2. Photo-catalysis using TiO_2 leads to the degradation of NO/NO_2, benzene, toluene, and other priority air pollutants once in contact with the semiconductor surface. The development of innovative coatings containing TiO_2 as a photocatalyst was in the foreground of research activities with the aim to be used as building and construction materials mainly outdoors, e.g. on building facades in high traffic roads for the degradation of priority air pollutants (NOx and volatile organic compounds) in the polluted urban atmosphere.

Though the advantages connected with the application of TiO_2 due to its band gap of 3.2 eV are limited. TiO_2 is effective only in the UV-region (5%) of the solar spectrum with wavelengths <380 nm. Hence, efforts made to increase the activity of TiO_2 using visible light, which will expand its application in indoor environments too. Many transition metals such as V, Cr, Fe, Mn, Ni, Co, Cu, Zn have been explored to reduce the energy gap and facilitate the transfer of electrons to the conduction band and thus extend the spectral range of modified TiO_2 to the area of visible light. In our experiments, 0.1% (w/w) and 1% (w/w) Mn-TiO_2 admixtures were prepared and the ability of the modified photo-catalysts to degrade NO by both solar and indoor illumination was evaluated.

The surface chemistry at the air/catalyst interface governed by the photoelectric characteristics of TiO_2 and the formation of reactive oxygen species with co-occurring redox reactions is reviewed and the factors affecting the application of TiO_2 for the degradation of priority air pollutants as single compounds or mixtures in ambient air and confined spaces are discussed.


SYNTETIC / ORGANIC
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DAY 2

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From conventional to green: Latest trends in fertilizer industry

C. Avşar, D. Tümük, N. Aka and **A.O. Gezerman**
Toros Agri Industry and Trade Co. Inc.,Turkey

Today, due to the global population increase and enhanced industrialization capacity, deplation risk of limited and unsustainable resources is a challange. Besides, continous anthropogenic and industrial activiy-based emissions have an accumulated impact on the concentration of greenhouse gases (GHGs), mostly CO_2, resulting the global warming and climate change issues. New terms such as Circular Economy, Sustainable Development, Green Deal, have been emerged to mitigate the negative effects of the climate change and to make the globe more sustainable for next generations.

Global population increase and as-related food demand is the most important driving force in the increased production capacity of mineral fertilizers, since fertilizers are the key factors to increase the agricultural yield. Conventional fertilizer production strategies are based on a linear-based economy and energy-intensive routes, utilizing fossil-fuel based feedstocks. The use of fossil fuels in the energy sector is still a necessity, but there are various initiatives for the use of renewable energy sources. At this point, there is a shift from conventional technologies to novel approaches towards renewable-based resources, which will play a strategic role in increasing energy efficiency in the agricultural industry and reducing the need for fossil fuel-based feedstocks. Incorporation of renewable resources in the conventional production routes might be a strategic approach to decrease the utilization rate of conventional feedstocks. As an example, green ammonia, although not widespread on the market yet, is an important breakthrough for the fertilizer industry to reduce the industry-specific contribution to GHGs emissions. Besides the potential modifications in the production routes, introducing circular economy strategies on the fertilizer formulations such as biostimulants, biochar, biomass etc. utilization might result low-carbon fertilizer products and approach to a greener industry. Mineral fertilizers are indispensable for high-yield and healthy growth in agriculture, however these fertilizers with modified formulations might be promising mates to mineral fertilizers to strengthen their nutritional effect even better with a lower environmental footprint.

Biography

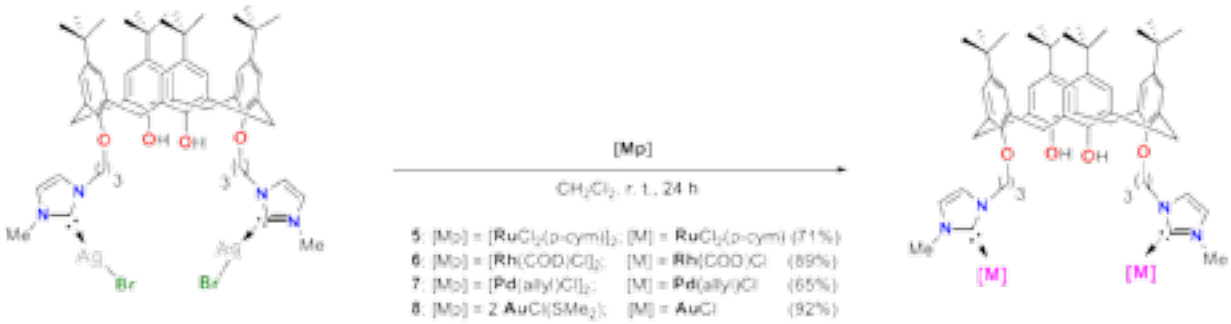
Cemre Avşar is a chemical engineer and currently works as a R&D specialist at Toros Agri Industry and Trade Co. Inc. R&D Department. She holds a BSc degree in chemical engineering from Gazi University, MSc degree in chemical engineering from Middle East Technical University, and currently a PhD candidate in chemical engineering at Ankara University. Her expertise lies in chemical engineering thermodynamics, process optimization in reaction kinetics, and phosphogypsum management and conducts experimental methodologies for the recycle routes and process optimizations in the mineral fertilizer industry. She is also the author/co-author of various studies on the recycling and evaluation of industrial wastes within the framework of the Green Deal concept, green ammonia, an alternative energy source with zero-carbon emission to fossil fuels, and the use of new generation nanomaterials as an alternative to the phosphate fertilizers used in agriculture published in various international journals.

Synthesis and catalytic applications of metal complexes supported by NHC-based cyclophanes

D. Mendoza-Espinosa and **F. J. Ruiz-Mendoza**
Universidad Autónoma del Estado de Hidalgo, Área Académica de Química, Mineral de la Reforma, México

Calix[n]arenes are well known polyphenol macrocyclic structures which offer several advantages over other molecular systems including their relatively easy functionalization at their lower- and upper-rims, the presence of hydrophobic cavities, and the presence of flexible core/scaffolds that can be modified for target substrate binding. Their application in the design and synthesis of new ligands for metal ions is of current ongoing interest in supramolecular chemistry due to the roles that these ions play in biological, environmental, and chemical processes.

NHCs (N-heterocyclic Carbenes) rank among the most powerful ligands for transition metal catalyzed chemical transformations. Mesoionic carbenes (MICs) are a new class of ligands that have received considerable attention as they have been postulated as better sigma donors compared to their classical NHC counterparts. Owing to their synthetic versatility, a vast family of metal complexes bearing MICs has been reported in the literature, usually targeting their application in homogeneous catalysis. The increasing interest on cleaner chemical processes has risen attention in multi-metallic complexes owing to their superiority in terms of enhanced reactivity and selectivity compared to their monometallic counterparts. In recent years, our group has shown that multinuclear metal complexes of MICs can be used to generate highly potent catalysts for C-C cross-coupling reactions, hydrosilylations, cycloaddition reactions, among others. Designing conceptually new carbon- donor ligands, incorporating their strong donation properties, and developing hybrid platforms stabilized by macrocyclic frameworks (such as calixarenes) are current research topics in our laboratory. In the present work we describe the synthesis of novel hybrid calixarene NHC/MIC architectures and their use as ligands for the stabilization of metal complexes. The structural diversity in solution and solid state of all new complexes and their preliminary catalytic activities will be discussed.



Biography

Daniel Mendoza-Espinosa was born in Mexico City. He obtained his B. Sc. at Universidad Autonoma del Estado de Hidalgo (UAEH) and his Ph. D. in Chemistry at Texas Christian University. After two years of postdoctoral Research at University of California, San Diego under the supervision of Pr. Guy Bertrand, he returned to Mexico to work on TEVA Pharmaceuticals in the R&D department. In 2012, he moved to Mexico City to work as invited professor at Universidad Autonoma Metropolitana and since 2018, he is a Professor at the Chemistry Department of UAEH. His research involves the development of multinuclear metal complexes and their application in catalysis and to date, he has published more than 50 chemistry JCR articles. He is alumni of the 63rd Lindau Nobel Laureate Meeting (2013) and he has received the Early Chemist Award granted by the Pacific Basin Societies in the years of 2015 and 2021.

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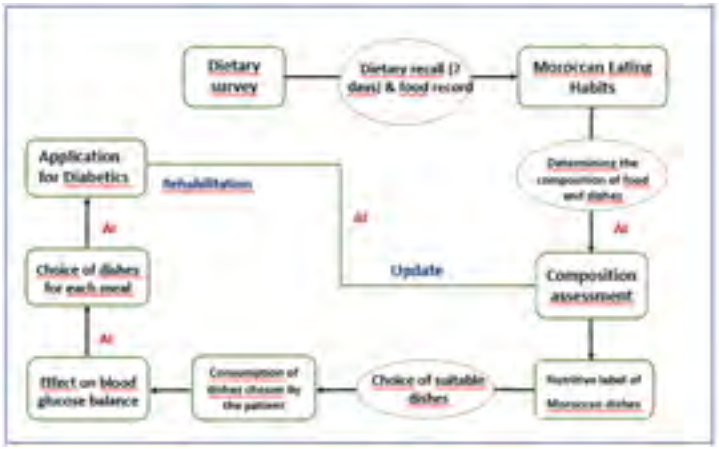
Artificial intelligence applied to nutritional therapy in Moroccan type 2 diabetics: Methodological approach

S.Chellak[1], K. E.Moutaouakil[2], M. Cheggour[1] and **H.Baizri[3]**

[1]Morphosciences Research Laboratory, Faculty of Medecine and Pharmacy, Cadi Ayyad University of Marrakech, Morocco
[2]Engeneering Science Laboratory, Faculty Polydisciplinary of Taza, Sidi Mohammed Ben Abdellah University of Fès, Morocco
[3]Bioscience and Health Laboratory, Faculty of Medecine and Pharmacy, Cadi Ayyad University of Marrakech, Morocco

This work aims to present the research project funded by two Moroccan national authorities: the national center for scientific and technical research and the digital development agency. Its main goal is to develop an application based on artificial intelligence that will help Moroccan type 2 diabetics to better choose their meals by helping them to balance their blood sugar. To achieve this, several steps are planned.

At first a food survey was conducted in different regions of Morocco in order to select the most consumed moroccan dishes and determine their composition in nutrients. Also, we have already integrated the principles of modeling and machine-learning, in particular to classify foods and their composition, to determine the nutrient needs of individuals and also to propose a multi-objectives optimal control model to control a population of diabetics taking into account the specificity according to their degree of complication and their response to the proposed diets.



Representative diagram of the methodological approach

Biography

Ms. Saliha CHELLAK
Pharmacist Biologist
Head of the Laboratories Division.
Avicenna Military Hospital - Marrakech
Professor of Chemistry – Biochemistry.
Faculty of Medicine and Pharmacy.
Cadi Ayyad University – Marrakech

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Lithium ions extraction from sea water bittern using room temperature ionic liquid

A. Hormati[1] and **N. Pourmand**[2]

[1]*CEO Manager of the First Producer of Industrial Salt from Sea Water in Iran (Khak Ab Sazeh), Iran*
[2]*PhD of Analytical Chemistry, Research Manager of Khak Ab Sazeh and Dolphin Sea Salt Company, Iran*

Sea water bitterns (SWB) are produced in the processes of desalination and sea-salt production where large quantities of bitterns and brines are produced as by-products. SWB remains after evaporation and crystallization of sodium chloride (table salt) from brines and sea water, it was reasonable to think of solar evaporation as the cheapest and most economical means for the preconcentration of sea-bittern. Lithium (Li) procurement is becoming a matter of importance worldwide. Lithium plays an important role currently in ceramic, nuclear power, aerospace, military industries, lithium batteries, metallurgy, medicine and so on. Recently, more attention has been given to use ionic liquids (ILs) in lithium solvent extraction, which is efficiently and successfully recovery of lithium from Sea water bitterns. Room temperature ILs are very ofordable and green alternative to organic solvents in classical extraction techniques and good candidate to replacing with organic solvents as green alternatives for microextraction studies. In this study a simple dispersive liquid–liquid micro extraction methods based on plain ILs-DLLME combined with inductively coupled plasma optical emission spectrometry (ICP-OES) was applied for extraction and determination of lithium from Sea water bitterns by employing tributyl phosphate (TBP) and 1-hexyl-3-methylimidazolium [C6mim+] as cation and bis(trifluoromethylsulfonyl)imide [NTf2-] as anion of ionic liquid (ILs). The extraction of Li was proceeded by solvation of Li with TBP followed by cation exchange with the ionic liquid. The effective parameters on lithium ions extraction process were studied including solution pH (~7), adsorbent dosage (100 & 300 mg) and extraction time (30 & 120 min). The extraction efficiency of lithium ion was more than 90% for ILs under the optimal conditions.

Biography

Abdolreza Hormati is CEO Manager of the first producer of industrial salt from sea water in Iran. He received a bachelor's degree in mining engineering in 1993 from Shahrood University of Technology, Iran and a master's degree in mineral processing engineering in 2012, Yazd Azad University, Iran and currently he is PhD student in mining engineering from science and research branch of Islamic Azad University, Tehran, Iran. From 1997 to 2022, he has been working professionally in the production of industrial salt from sea water to supply the petrochemical industries of chloralkali units in Khuzestan, South of Iran. He with his R&D team has conducted extensive studies on the new methods of producing potassium sulfate - magnesium sulfate - magnesium chloride - magnesium hydroxide and lithium production from sea water.

Neda Pourmand is the research and development manager of the Khak Ab Sazeh and Dolphin sea salt company. She received a PhD degree of analytical chemistry from Universiti Teknologi Malaysia (UTM), Malaysia and from 2018 until now, she has been working on recovery valuable materials from sea water.

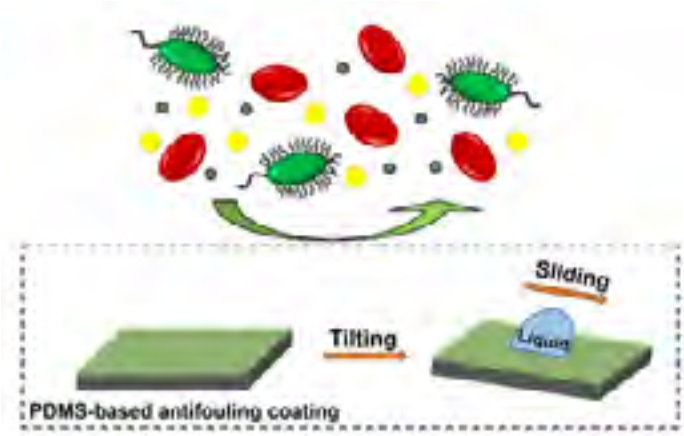
Preparation and characterization of PDMS-based antifouling coatings

Esra Kasapgil

Izmir Bakircay University, Turkey

The term "fouling" refers to a cumulation and encrustation process of unwanted substances from the environment to the surface of a material. These unwanted foulants can be dirt, sand, rust, oxide layer, mineral salts, colloids etc. Besides, biological foulants such as microorganisms, bacteria, proteins, etc. can be adhere to the surface and cause biofilm formation and biofouling. Fouling/ biofouling is an undesired situation that causes failure and capacity loss of materials or devices. To overcome this problem, antifouling coating technologies are being developed. Understanding the surface shape, chemistry, heterogeneity and superhydrophobicity/ superhydrophilicity is essential for developing antifouling strategies.

Superhydrophobic surfaces have attracting researchers due to their excellent properties such as anti-fouling, anti-icing, and self-cleaning. On the other hand, slippery liquid infused porous surfaces (SLIPS) are a developing class of self-cleaning surfaces with high anti-fouling and multi-liquid repellency properties. In this work, polydimethylsiloxane (PDMS)-based superhydrophobic coatings and SLIPS were prepared on different substrates. Both coatings have high liquid repellency against water and oil-based liquids. The durability of coatings against raining conditions, heating conditions and acidic/basic solutions were compared, and it was found that both coatings were durable. The aim of this work is to present the results of obtained PDMS-based superhydrophobic coatings and PDMS-based SLIPS as antifouling coating candidates and the possibilities of using these coatings in different applications.



Schematic illustration of the repellency property of PDMS-based antifouling coatings.

Biography

Esra Kasapgil obtained her bachelor's degrees in Chemical Engineering and Metallurgical and Materials Engineering from Istanbul Technical University, Turkey in 2012 and her master's degree in Materials Science and Engineering from the same university in 2014. In 2020, she obtained her Ph.D. degree in Materials Science and Engineering from Gebze Technical University in Turkey where she had also worked as a research assistant in 2013-2020. During her PhD studies she focused on coating technologies, polymeric thin films, bio-inspired superhydrophobic surfaces and slippery liquid infused porous surfaces (SLIPS) for self-cleaning and antibiofouling applications. She was a visiting researcher in Biomedical Engineering at McMaster University, Canada in 2019-2020. Esra is currently an Assistant Professor in the Department of Biomedical Engineering at Izmir Bakircay University, Turkey. Her research interests are coating technologies, thin film technologies, superhydrophobic coatings, antifouling coatings, surface modification of biomaterials, polymer chemistry, polymer synthesis and characterization, bioinspired materials and technologies.

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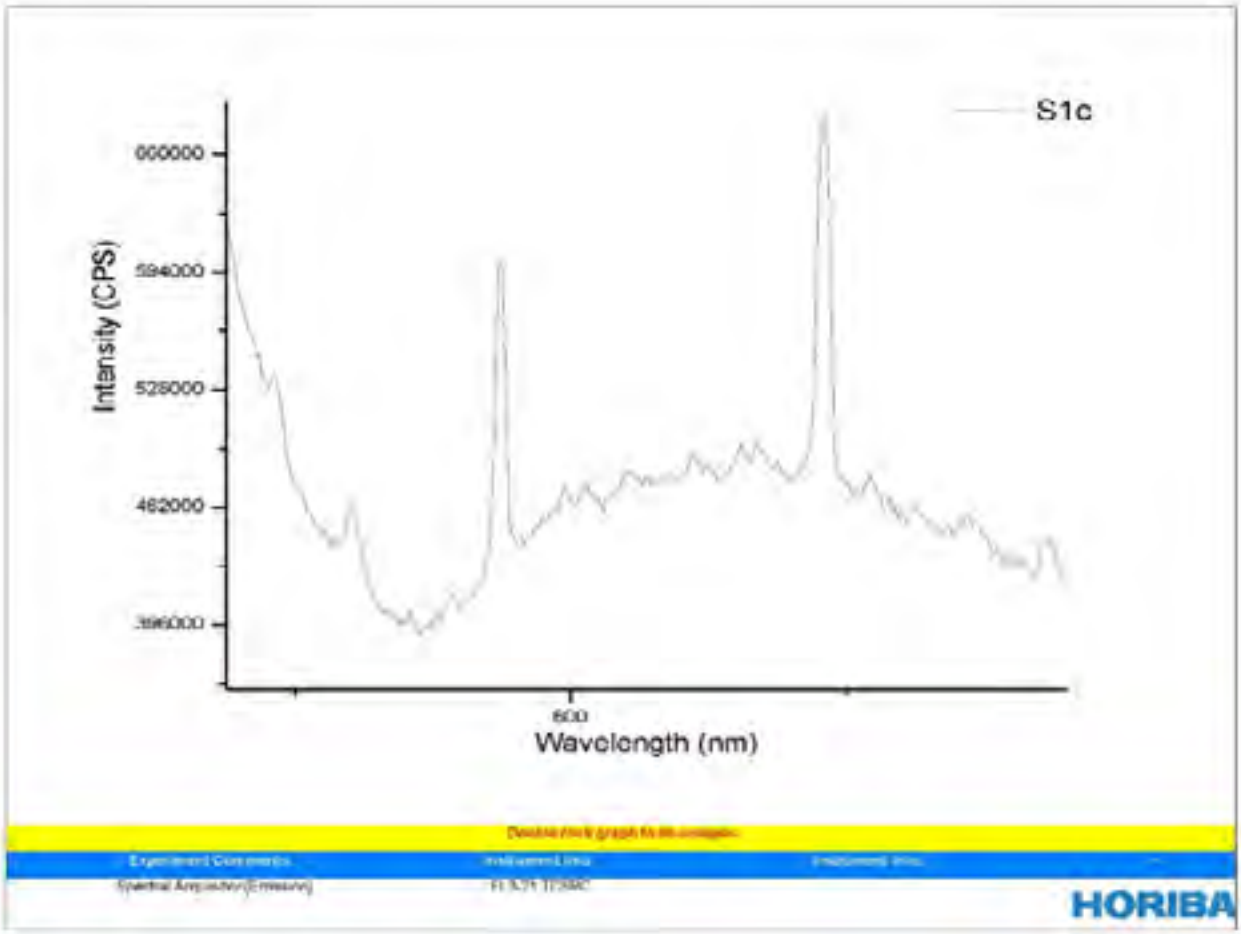
Structural and photoluminescence studies of microwave sintered $Ce_{0.8}Y_{0.1}Dy_{0.1}O_{2-\delta}$ solid electrolyte for IT-SOFC applications

Ch. Madhusudan[2] and
Kasarapu Venkataramana[1]

[1]*Department of Humanities & Science, Keshav Memorial Engineering College, India*
[2]*Department of Physics, Government Degree College (A), India*

Oxygen vacancies are one of the most active defects, which attributes many important properties to the host lattice Ceria. Engineering of defect chemistry, especially oxygen vacancies, represents the possibility of controlling various electrolytic, catalytic, and optical properties of Ceria nanoparticles. Y and Dy co-doped ceria i.e. $Ce_{0.8}Y_{0.1}Dy_{0.1}O_{2-\delta}$ (CYD) was prepared by sol-gel auto-combustion technique. Prepared sample was sintered at 1300°C for 4h by microwave sintering approach. X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), and other techniques were used to examine the structural, morphological, elemental, and optical characteristics of synthesized sample. The single phase and cubic structure were confirmed by the powder X-ray diffraction (PXRD). Relative density of CYD was found to above 95% of the theoretical value. Surface-microstructure analysis of CYD sample was studied by scanning electron microscopy (SEM). X-ray Photoelectron Spectroscopy (XPS) results confirmed the incorporation of Y and Dy in the ceria crystal lattice. XPS results also indicated the co-existence of Ce^{3+} and Ce^{4+} states, offering co-doped ceria with a higher concentration of oxygen vacancies. Photoluminescence spectroscopy (PL) results of CYD revealed that the co-doping shifts the photoluminescence in the low energy range and lead to an intense photoluminescence emission. The results provide a valuable route for the rational design of co-doped ceria nanoparticles with the desired oxygen vacancy population, and then preparing them in the best conditions for various applications.



PL spectrum of CYD10

Biography

Dr. Ch Madhusudan was born in Telangana, India. He received his B.Sc. degree (in Physical Sciences) and M.Sc. (Physics) from Osmania University, Hyderabad. He did his Ph.D. in Physics on "Electrolyte Materials for Intermediate Temperature Solid Oxide Fuel Cells (ITSOFCs)" from Osmania University.

He was appointed as Assistant Professor of physics in Collegiate Education, Government of Telangana State, India. Currently he is working as Head of Department of Physics at Government Degree College, Siddipet (Autonomous), Telangana, and has been guiding UG/PG physics students in research projects. His main research area is Material Science. He has published several papers in reputed international journals and presented papers in National & International conferences. He has authored four ISBN books in Physics.

Dr. Madhusudan is a member of Indian science Congress, IEEE, Indian Association of Physics Teachers (IAPT). In the capacity of IAPT Telangana State VP, he has been organising numerous Science Promotion activities/Workshops.

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Eco-friendly synthesis and application of tin sulfide

A. Bronusiene and **I. Ancutiene**
Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Lithuania

An odd synthesis of thin tin sulfide film preparation directly from abundant and biodegradable precursors via a simple "SILAR" method. One of the most challenging challenges is the development of thin films based on an inexpensive and simple process using materials of high abundance. It is very important to find cheap, environmentally friendly products that have the possibility of deposition in a large area and adhere well to the substrate method. The aim of the work was to form "environmentally friendly" thin tin sulfide films by applying the safety and inexpensive SILAR method and using "green" precursors, aqueous solutions, low deposition temperature, and environmental safety reducing agent. Biodegradable L-ascorbic acid was used as a reducing and capping agent for the synthesis. Deposited films were characterized for "supercapacitor" application.

The films obtained were uniform, without any damage, and visible pinholes, also, well adhered to the substrate. The obtained SnS was considered to have an orthorhombic crystal structure. Mineral "herzenbergite" is assigned to the peaks of the deposited material. Raman analysis together with XRD confirms the growth of single-phase SnS. The annealing of the deposited films improves the morphology and compactness of the films. Here "nanoparticles" were obtained with a size between 9-30 nm. The bandgap values of the deposited films are very close to the theoretical values of herzenbergite. The initial electrochemical testing of cyclic voltammetry and galvanostatic charge-discharge cycling was performed. The shapes of both CV and GCD curves signify a dual charge storing mechanism. Tin sulfide thermally treated at 300 ° C should be possessed as the most active with respect to its current response to applied potential. Since its composition is presumably the same, other parameters, such as morphology and porosity, may be determining factors.

In this current work we described a facile, eco-friendly technique to synthesize L-ascorbate acid stabilized tin sulfide nanoparticles. The results exhibited that the SnS thin films after annealing demonstrate possibility for use in electrochemical capacitors.

Biography

I am a Ph.D. student at Kaunas University of Technology in the Department of Physical and Inorganic Chemistry. Bachelor of Chemistry received from Kaunas University of Technology in 2014. The theme was copper sulfide preparation. In master's years, molybdenum sulfides were prepared on glass slides. Ph.D. studies started in 2018 and have a break due to maternity leave for one year in 2020-2021. During Ph.D. studies, thin films of tin sulfides on electric-conductive glass slides were prepared. The applications of tin sulfide in supercapacitors and solar cells were investigated. Furthermore, it was pioneering TiO2 deposition and solar cell preparation in the Physical and Inorganic Chemistry Department. During whole masters and Ph.D. years worked in inorganic chemistry laboratory with students. This involves not only the preparation of laboratory tests, also discussions with students. Now 6 articles are printed and attended 14 conferences. Still working with chalcogens, deepening skills in application fields.

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Selenium speciation analysis in lactic acid bacteria cultivated under stress conditions

Vera Nesporova[1], Ivana Hyrslova[2], Gabriela Krausova[2] and **Antonin Kana[1]**

[1]University of Chemistry and Technology, Czech Republic
[2]Dairy Research Institute, Ltd., Czech Republic

Deficiency of selenium in human diet is still one of the current topics in the field of nutrition related research. Lack of this essential nutrient is observed in many countries, including Czech Republic. To avoid the traditional concept of food supplements as pills, we came up with a different approach. Lactic acid bacteria are widely used in dairy industry and are generally recognized as safe. Moreover, fermented dairy products, such as yoghurt, kefir, sour cream, etc. are beneficial for human digestive tract itself. Lactic acid bacteria (e.g. *Streptococcus, Lactococcus and Enterococcus* genera) shows good ability to incorporate and biotransform inorganic selenite into organic species (e.g. selenomethionine, selenocystine, methylselenocysteine) or elemental nanoparticles, after being cultivated in Se-enriched growth media. This ability is well described by many authors for optimal conditions of cultivation, however the influence of stress conditions hasn´t been described yet. In our study, we analyzed the CCDM 144 *Streptococcus thermophilus* bacterial strain under 3 different cultivation temperatures (25°C, 35°C, 45°C, namely). Firstly we determined the total selenium content in freeze-dried sample after the microwave-assisted digestion by ICP-MS. Secondly, the samples were extracted by proteinase XXIII in Tris buffer, prior to speciation analysis realized by ion-pair liquid chromatography. Lastly, the samples were dispergated in 1% methanol solution prior to sp-ICP-MS analysis to determine the content of selenium in nanoparticles. The results confirmed the premise of different behavior of bacteria under stress conditions. As expected, the highest temperature (45°C) caused the biggest increase of accumulated selenium. In case of total Se content we observed almost 3-fold increase of accumulated selenium. Similar trends were observed in speciation. The content of major specie, selenocystine, doubled its amount at 45°C. On the other hand, methylselenocysteine decreased three times compared to 25°C and even four times for 35°C. Results obtained from analysis of nanoparticles are in accordance with trends mentioned above. The production of nanoparticles increased under the stressed condition, and, also the particle diameter was magnified.

Biography

Vera Nesporova (Kantorova) is a 3rd year Ph.D. student at the University of Chemistry and Technology in Prague. Since the bachelor´s she studies at Department of Analytical chemistry in the group of Atomic Spectrometry, focusing on ICP-MS. The aim of her doctoral thesis is speciation analysis (coupling of HPLC to ICP-MS) of selenized probiotic cultures (lactic acid bacteria, bifidobacteria and yeast), and its possible usage as a functional food. She is an author/co-author of 5 impacted articles. For many years, her hobby is cheerleading, she´s been coaching the Prague Eagles for 9 years, after ending active career. Her other passion is the family cat named "Biscuit".

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Relationship among *Blastocystis*, the *Firmicutes/Bacteroidetes* ratio and chronic stress in Mexican University students

Iliana Itzel Lozano-Ochoa, Janeth Oliva Guangorena-Gómez, Ilse Lizeth Rivera-Medina, Alejandra Méndez-Hernández, Jorge Antonio Espinosa-Fematt and **Claudia Muñoz-Yanez**

Universidad Juarez del Estado de Durango, Mexico

The role played by *Blastocystis* in humans has been a subject of discussion due to its intestinal effects and modifications in the intestinal microbiota. We aimed to analyze the relationship between *Blastocystis* subtypes ST1-4 and 7, the Firmicutes to Bacteroidetes ratio (*F/B* ratio) of fecal microbiota, and chronic stress in university students. This study had a cross-sectional design with a sample of 202 students. We analyzed fecal and hair samples, and stress inventories were applied to the stu- dents. The results showed a frequency of Blastocystis-colonized students of 52.97%. Regarding fecal microbiota, a median RAU of 0.801 for Firmicutes and 0.82 of Bacteroidetes were obtained, with an *F/B* ratio of 0.83. A low *F/B* ratio (66.04%) was more frequent in Blastocystis-colonized students, whereas a high *F/B* ratio (68.09%) (p = < 0.0001) was found in the Blastocystis-non-colonized. Only *Blastocystis* ST3 did not significantly correlate with a low F/B ratio (p = 0.290). The ST4 was associated with lower values of cortisol (p = 0.030), psychological stress (p = 0.040), and lower frequency of constipa- tion (p = 0.010). Only two students with the ST1 had abdominal pain (p = 0.007). Our results suggest that colonization by *Blastocystis* subtypes can modify the intestinal microbiota due to a decreased ratio between the two most representative phyla (*F/B*). Also, the results of this study show that ST4 colonization is related to a lower level of chronic stress.

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March 27-28, 2023 | Barcelona, Spain

Development of nimesulide analogs as a dual inhibitor targeting tubulin and HSP27 for treatment of female cancers

Laila A. Jaragh-Alhadad[1], Gamaleldin I. Harisa[2,3,4] and **Fars K. Alanazi[2,3]**

[1]Department of Chemistry, College of Science, Kuwait University, Kuwait
[2]Kayyali Chair for Pharmaceutical Industry, College of Pharmacy, King Saud University, Saudi Arabia
[3]Department of Pharmaceutics, College of Pharmacy, King Saud University, Saudi Arabia
[4]Department of Biochemistry and Molecular Biology, College of Pharmacy, Al-Azhar University, Egypt

In the drug repurposing paradigm, medicines that are already used to treat the specific diseases can also treat alternative ones. Recently, nimesulide was reported as an antitumor agent, besides its anti-inflammatory effect. Tubulin and heat shock protein 27 (HSP27) are attractive targets for the discovery of anticancer therapy because both are upregulated in cancer cells. In this regard, this study aims to develop the nimesulide skeleton, synthesize, characterize, and biologically evaluate the new nimesulide analogs as anti-cancer agents through the inhibition of tubulin and HSP27 functions. The synthesized agents were characterized by 1H NMR, 13C NMR, IR, melting point and both endothermic and exothermic DSC analysis. The molecular weight was confirmed using GC–MS technique. N-(3-((2,5-dichlorobenzyl) oxy)-4-(Nmethylmethylsulfonamido)phenyl)-4-iodobenzamide (agent L4) structure was confirmed using X-ray crystallographic analysis. The ligands adopt triclinic crystal with a = 8.194(14) A, ° b = 10.75(3) A, ° c = 14.21(2) A° and space group of P-1. Western blot analysis was used to express the presence of the dual proteins on the harvested SKOV3 and SKBR3 cell lines. The anticancer effect of nimesulide analogs was studied using MTT assay on SKOV3 and SKBR3 cell lines as a surrogate model for ovarian cancer, and breast cancer respectively. The present results indicated that the developed nimesulide analogs elicited cytotoxicity against SKOV3 and SKBR3 cell lines in turn cell cycle arrest, in the concentration range between 0.23–2.02 µM and 0.50–3.73 µM respectively. This study concluded that nimesulide analogs are potent promising agents for the repurposing of nimesulide as future chemotherapy for female cancers.

Biography

Dr. Laila Jaragh-Alhadad research's interest focuses on design, synthesis, characterizing & biologically evaluation of anticancer agents that target small molecules which have essential role and their levels encouraging cancer cell division. The first project area is targeting both HSP27 & HER2 proteins with inhibitors in several human cancer cell lines to improve the ADME profile. HSP27 and HER2 proteins are attractive molecular targets for cancer therapy because of their cellular functions, proportionally up-regulated in cancer cells. The goal is to synthesize a library of compounds targeting HSP27 and stabilize HER2 through the HER2 pathway and choose the best drug candidate for further in-vivo evaluations. The development of this series of anticancer agents may overcome the chemotherapy drug resistance and improve the survival of cancer patients. The second project area is drug delivery strategy to cancer cells, to accumulate a certain amount of the drug to some part of the body relative to others. The goal is to encapsulate the drug candidate into nanoparticles such as low-density lipoprotein, liposomes & cholesterol conjugates to mimic the natural lipid metabolic pathway to reach the center of cancer cells, improve the drug efficacy, delivery, and minimize toxicity side effects. In addition, targeting tubulin structural protein that has important cellular roles in cell proliferation with anticancer agent to inhibit cancer cells growth. Generally, benefits from drugs already in the market and apply structure activity relationship to the drug skeleton to convert them to anticancer drugs useful for cancer patients' treatment.

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Association study of HIF-1α rs11549465 and VEGF rs3025039 genetic variants with diabetic retinopathy in Egyptian patients: Crosslinks with angiogenic, inflammatory, and anti-inflammatory markers

Leqaa A. Moemen[1], Mahmoud K. Mohamed[1], Azza A. Atef[2], Amira A. Abdel Azeem[1], Islam A. Mohalhal[1] and **AlShaimaa M. Taha[2]**

[1]Research Institute of Ophthalmology, Egypt
[2]Faculty of Science, Ain Shams University, Egypt

Background: Genetic factors are implicated in the progression of DR; a global cause of blindness. Hence, the current work investigated the association of HIF-1α rs11549465 and VEGF rs3025039 genetic variants with the different stages of retinopathy among T2DM Egyptian patients. The crosslinks of these variants were explored with angiogenesis (VEGF), inflammation (AGEP and VCAM-1), and anti-inflammation (CTRP3) markers. 288 subjects were recruited in this study: 72 served as controls and 216 were having T2DM who were divided into diabetics without retinopathy (DWR), diabetics with non-proliferative retinopathy (NPDR), and diabetics with proliferative retinopathy (PDR). The genetic variants were analyzed using PCR-RFLP and their associations with NPDR and PDR were statistically tested. The circulating levels of AGEP, VCAM-1, HIF-1α, VEGF, and CTRP3 were assayed followed by analyzing their associations statistically with the studied variants.

Results: Only HIF-1α rs11549465 genetic variant (recessive model) was significantly associated with the development of NPDR among T2DM patients ($p < 0.025$) with a significant correlation with the circulating HIF-1α level ($p < 0.0001$). However, this variant was not associated with PDR progression. Neither HIF-1α rs11549465 nor VEGF rs3025039 genetic variants were associated with the PDR progression. The circulating AGEP, VCAM-1, HIF-1α, VEGF were significantly elevated ($p < 0.0001$) while the CTRP3 was significantly decreased ($p < 0.0001$) in NPDR and PDR groups. The HIF-1α rs11549465 CT and/or TT genotype carriers were significantly associated with AGEP and VCAM-1 levels in the NPDR group, while it showed a significant association with the CTRP3 level in the PDR group. The VEGF rs3025039 CT genotype carriers showed only a significant association with the CTRP3 level in the PDR group.

Conclusion: The significant association of HIF-1α rs11549465 other than VEGF rs3025039 with the initiation of NPDR in T2DM Egyptian patients might protect them from progression to the proliferative stage via elevating circulating HIF-1α. However, this protective role was not enough to prevent the development of NPDR because of enhancing angiogenesis and inflammation together with suppressing anti-inflammation. The non-significant association of HIF-1α rs11549465 with PDR among T2DM patients could not make this variant a risk factor for PDR progression.

Biography

- Professor in Medical Biochemistry Unit - RIO, June, 2004.
- MD in Medical Biochemistry, Faculty of Medicine, Cairo University, November, 1993.
- Manager of (RIO - Knowledge transferee technology office).
- Member of: Egyptian Society of Biochemistry and Molecular Biology,

Conferences:

- The Annual Meeting of Association for Research in Vision and Ophthalmology, (4-8 May, 2003), Fort Lauderdale, Florida. USA – for third time.
- The Annual meeting of European Research in Ophthalmology and Vision, (7-10 October, 1998), Palma de Mallorca, Spain.

Workshops:

- Knowledge & Technology Transfer at LURIS, Leiden University, the Netherlands on the 22nd 24th of October 2019 .
- Effective academic writing, Nov 2019.By Nature research Academics. Cairo, Egypt.
- Clinical research methodology, Sep 2019. Nature research Academics. Cairo, Egypt.

Scientific Activity:

- Member of the Standing Committee of the promotion upgrades from 2012-2015.

Scopus ID: 34168147400

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A 4-year of HbA1C assay performance from Thailand in the European HbA1c Trial

Supaporn Suparak[1], Kanokwan Ngueanchanthong[1], Petai Unpol[1], Ariya Thanomsakyuth[2], Chavachol Setthaudom[2], BusadeePratumvinit[3], Mongkol Kunakorn[2] and **Archawin Rojanawiwat[1]**

[1]Department of Medical Sciences, Ministry of Public Health, Thailand
[2]Faculty of Medicine Ramathibodi Hospital, Thailand
[3]Faculty of Medicine Siriraj Hospital, Mahidol University, Thailand

Background: Thailand National External Quality Assessment organiser for HbA1c was participated in the EurA1, European HbA1c Trial since 2018, so far 25 EQA organisers of 21 countries agreed to participate. Fresh whole blood and lyophilized hemolysate specimens manufactured from the same pool were used to evaluate analytical performance of the laboratories according to criteria of the International Federation of Clinical Chemistry and Laboratory Medicine (IFCC) model for quality targets.

Methods: 14 organisers including Thailand used lyophilised hemolysate samples for HbA1C evaluation. HbA1c results from laboratories were compared to the target value, the mean of the Secondary Reference Measurement (SRM) values as measured with the IFCC calibrated secondary Reference Measurement Procedures. Results of all countries are evaluated and presented in terms of performances per country and per manufacturer.

Results: During 2018-2021, at the country level tested with lyophilized hemolysates, 5-10 countries met the criterion (bias ≤ 2 mmol/mol and between laboratory CVs ≤ 6%) and 4-9 did not. The overall mean bias was 0.4 to 1.1 mmol/mol and the between laboratory CV was 5.8 to 6.9 %. In Thailand, 134 -185 participating laboratories (excluded lab with %difference > ±25), the mean bias of HbA1c ranged between -2.0 to 0.7 mmol/mol. The overall coefficients of variation ranged from 7.6 to 10.1%. The pass rates were 57.45 to 80.12% (% difference within ±8.00 %). Result per manufacture, there was 1, 0, 2 and 1 manufacturers met the criterion, in 2018 - 2021, respectively (bias ≤ 2 mmol/mol).

Conclusions: Performance evaluation in the European HbA1c Trial and in Thailand indicated that results per manufacturer/ per EQA organiser had an effect on HbA1c analysis. The major contribution to total error derived from between-laboratory variation. Participating in the external quality assessment programs is an effective educational tool for monitoring the quality of HbA1C testing and laboratories.

Biography

Professional positions:

- B.Sc. (Medical technologist), M.Sc. (Immunology), Ph.D. (Immunolgy)
- Medical Technologist, Senior Professional level, Department of Medical Sciences, Ministry of Public Health, Thailand.

Experience: Responsible for provide External Quality Assessment of laboratory testing on HbA1c testing and transfusion-transmitted pathogens. Co-operative and supportive actions on HbA1c testing in Thailand and provide quality assurance procedures for HbA1c laboratory network to other agencies, both domestic and international.

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Resilience of glass fiber-modified advanced polymer composites

Catherine Vasnetsov, Luis Rodriguez and **Victor Vasnetsov**

Caribbean Environment and Development Institute, Puerto Rico

Synthetic thermoplastic polymers have a highly attractive spectrum of physical properties: light weight, low cost, flexibility in processing, however, they have low physical strength. Addition of synthetic inorganic fibers (glass, ceramic, carbon) improves both thermal and dimensional stability of plastic parts. This paper presents results of stress-testing analysis as optimization enabler of composition for glass fiber-reinforced polymers using novel technology, including recycled polymers.

Advanced Fiber Reinforcements are continuous length reinforcing glass fibers embedded or encapsulated within thermoplastic resin (tensile strengths of 5,000 to 15,000 pounds per square inch). In contrast, glass fiber has a tensile strength 20-40 times more. This huge differential in tensile strengths can be very helpful when designing a larger molded part for challenging industrial applications, under continuous mechanical stress.

Our innovative method of reinforcement was proven to improve the strength of all rib designs by factor of several times; however, some rib designs show better improvement than others. The number of fiber filaments will also have a significant bearing on the amount of improvement of performance within a given rib design. During this research project, many different rib designs (i.e. length and width of a rib) were tested. A range of various rib designs (different rib heights and widths) was developed and tested utilizing reinforced plastic with 4,000, 8,000 and 12,000 glass fiber filaments and placed at the end of each rib. The molded test bars were tested in flex to optimize the ultimate flex strength improvement.

This poster will be presenting results of testing and optimization of the third generation of novel durable plastic pallets, which have highly positive environmental impact by replacing 70 times volume of short-lived virgin wood pallets. This is a rare and very powerful example how durable plastics actually save environment, instead of contributing to environmental problems.

Biography

Ms. Catherine Vasnetsov is a Student and a Research Associate at the Caribbean Environment and Development Institute at San Juan, Puerto Rico, where she has been working in extensive multi-year collaboration with ICP, an industrial plastics company.

Her research interests are focused on sustainable economic, industrial and social development, and the role of chemistry in creating innovative balanced solutions.

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A global consortium of the scientific fraternity, scholars, educationists, industry leaders and entrepreneurs to collaborate, share ideas and knowledge to resolve challenges across medicine, science, technology and business

Our Vision

"We aim to bring the research and innovations happening across the parts of the globe to facilitate interaction, knowledge sharing and exchange. We also aim to inspire university professors, students, researchers, clinicians and entrepreneurs from across the disciplines including but not limited to clinical, medical, business, technology, healthcare and pharmaceutical fields. Our dream is to bring advancements in the Science and Technology to the mankind through our scientific gatherings and deliberations. We believe in introducing novel methods and innovative techniques in science, business and technology to provide understanding on the developments".

Our Mission

How do we serve our target groups in the scientific & business community?

- We bring the untold research accessible for many.
- Our events meet the research needs of the target groups across the academia, industry, corporates, the government, non-government agencies and public bodies.
- We Engage. Enlighten. Empower people deprived of information.
- We connect the international giants towards finding simple solutions to the complex medical and healthcare challenges of the globe.
- We unveil the unlimited research opportunities to the sections of population that is away from the developments in science and technology.
- We encourage Young and emerging researchers and scholars.
- We extend continuous education credits to boost the career and academic progress.
- We encourage start-ups in science, technology and business for the social and economic empowerment of the enthusiastic entrepreneurs.

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INDEX

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