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4TH EDITION OF

Chemistry World Conference

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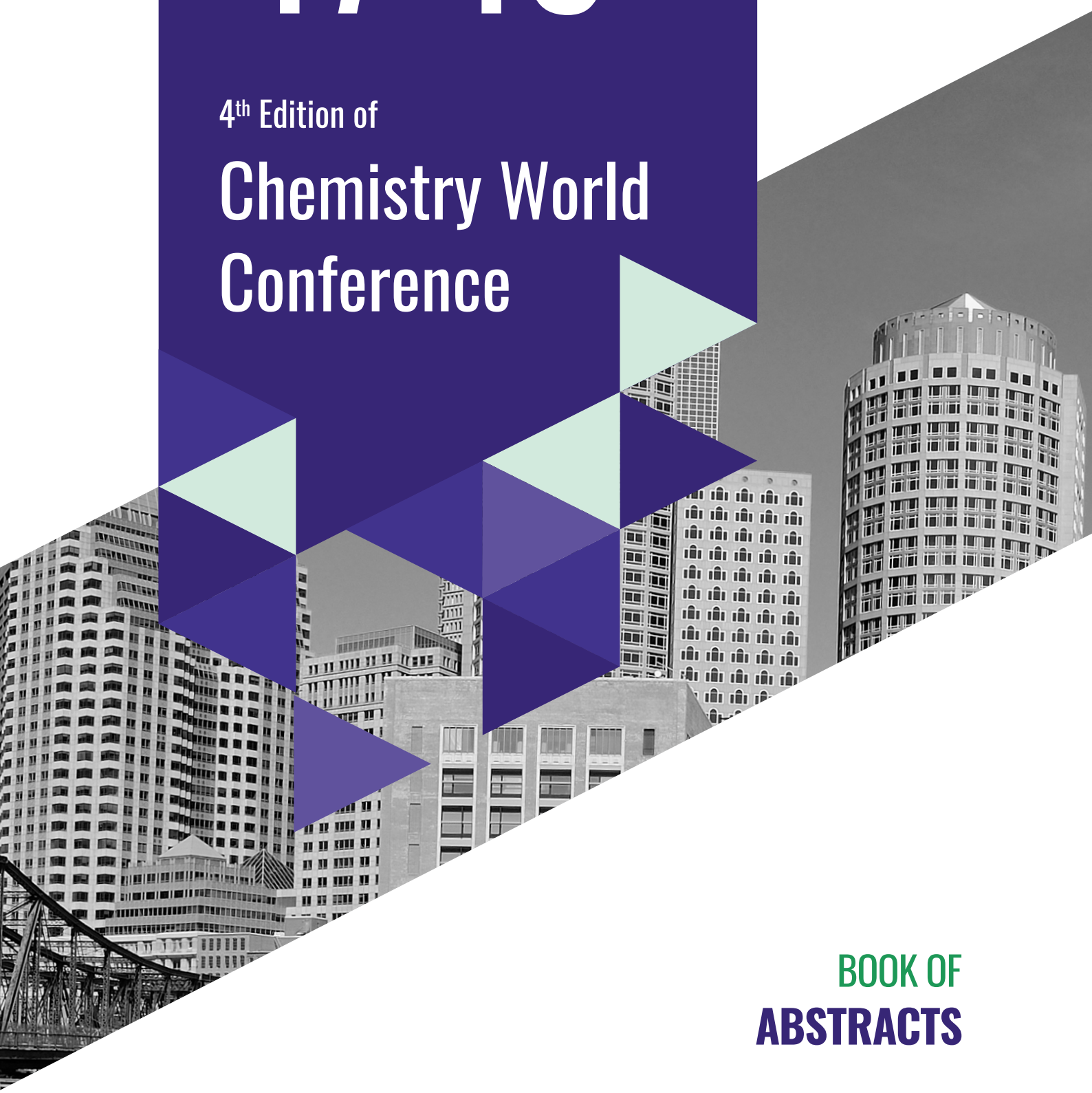
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JUNE

17-19

4th Edition of

Chemistry World Conference



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Brian S J Blagg
University of Notre Dame, United States



Haibo Ge
Texas Tech University, United States



Hossam A Gabbar
Ontario Tech University, Canada



Jean Maruani
Laboratoire de Chimie Physique - Matière et Rayonnement CNRS and Sorbonne-Universités, France



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Yong-Xiao Wang
Albany Medical College, United States

Thank You All...

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Thank You All...

Welcome Message



PROF. DR. YONG-XIAO WANG

Albany Medical College, United States

Dear Conference Visitors:

As the Conference Organizing Committee Member, I am very honored and pleased to write these welcome notes.

The current conference, Chemistry 2024, will bring together leading researchers, scientists, clinicians, and industry professionals from the chemistry field around the world to discuss the latest, energizing, and innovative developments as well as discoveries in **Evolutionizing chemistry to unveil breakthroughs and shape future objectives.**

Chemistry 2024 will include outstanding keynote sessions, plenary lectures, invited speeches, research presentations, technical demonstrations, and panel discussions around the world. One can expect that all these latest cutting-edge presentations and demonstrations will significantly advance almost all aspects from organic to inorganic chemistry to biochemistry to unique interdisciplinary studies.

I am very excited to look forward to meeting with you at this upcoming fantastic conference.



ABOUT
MAGNUS GROUP

Magnus Group, a distinguished scientific event organizer, has been at the forefront of fostering knowledge exchange and collaboration since its inception in 2015. With a steadfast commitment to the ethos of Share, receive, grow, Magnus Group has successfully organized over 200 conferences spanning diverse fields, including Healthcare, Medical, Pharmaceutics, Chemistry, Nursing, Agriculture, and Plant Sciences.

The core philosophy of Magnus Group revolves around creating dynamic platforms that facilitate the exchange of cutting-edge research, insights, and innovations within the global scientific community. By bringing together experts, scholars, and professionals from various disciplines, Magnus Group cultivates an environment conducive to intellectual discourse, networking, and interdisciplinary collaboration.

Magnus Group's unwavering dedication to organizing impactful scientific events has positioned it as a key player in the global scientific community. By adhering to the motto of Share, receive, grow, Magnus Group continues to contribute significantly to the advancement of knowledge and the development of innovative solutions in various scientific domains.



ABOUT
Chemistry 2024

4th Edition of Chemistry World Conference is a prestigious global event taking place in **Paris, France** from **June 17- 19, 2024**. Chemistry Events brings together scientists, researchers, chemists, chemical engineers, and industry professionals to exchange knowledge and explore advancements in chemistry. Chemistry Summit revolves around the theme ***Evolutionizing Chemistry: Unveiling Breakthroughs to Shape Future Objectives.*** It emphasizes the critical role of chemistry in material science, engineering, biology, and environmental science. Aim of Chemistry 2024 is to address contemporary challenges faced by societies worldwide and find innovative solutions.

Attendees can expect a comprehensive agenda with keynote sessions, workshops, oral and poster presentations, and networking events. Renowned speakers from academia, industry, and research institutions will share expertise on cutting-edge research, emerging trends, and breakthrough technologies in the field of chemistry. Chemistry 2024 Conference offers a unique opportunity for meaningful discussions, experience sharing, and establishing professional connections. Chemistry Meetings brings together like-minded individuals from around the globe, fostering collaboration and interdisciplinary discussions to shape a promising future for humanity through chemistry and allied fields.



ABOUT
CPD Accreditation

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Continuing Professional Development (CPD) credits are valuable for Chemistry 2024 attendees as they provide recognition and validation of their ongoing learning and professional development.

The number of CPD credits that can be earned is typically based on the number of sessions attended. You have an opportunity to avail 1 CPD credit for each hour of Attendance.

Some benefits of CPD credits include:

1. **Career advancement:** CPD credits demonstrate a commitment to ongoing learning and professional development, which can enhance one's reputation and increase chances of career advancement.
2. **Maintenance of professional credentials:** Many professions require a minimum number of CPD credits to maintain their certification or license.
3. **Increased knowledge:** Attending Chemistry 2024 and earning CPD credits can help attendees stay current with the latest developments and advancements in their field.
4. **Networking opportunities:** Chemistry 2024 Conference provide opportunities for attendees to network with peers and experts, expanding their professional network and building relationships with potential collaborators.

Note: Each conference attendee will receive 21 CPD credits.

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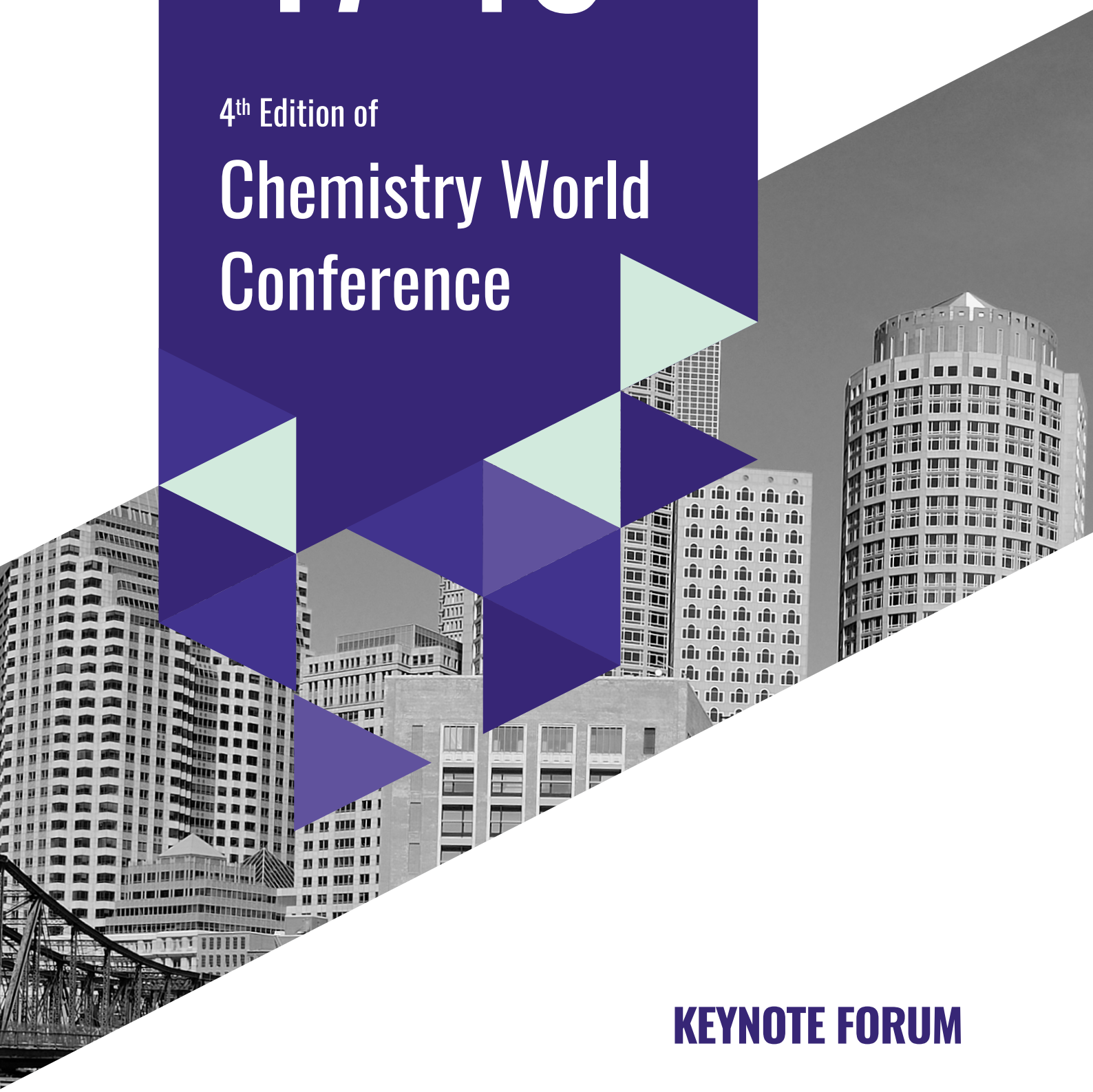
BOOK OF ABSTRACTS

JUNE

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KEYNOTE FORUM

The design and development of isoform-selective inhibitors of Hsp90

The Hsp90 molecular chaperone is composed of four family members that play key roles in the folding of nascent polypeptides as well as the rematuration of misfolded proteins. The cytostolic chaperones, Hsp90a and Hsp90b, contribute to tumorogenesis and represent attractive targets for the treatment of cancer. Grp94 is the ER-localized paralog that is responsible for the trafficking of proteins, such as myocillin, and consequently represents an ideal target for the treatment of primary open angle glaucoma. In contrast to the inhibition of Hsp90, the molecular chaperones can be overexpressed to exhibit neuroprotective activity in animal models of neuropathy. While the Hsp90 isoforms play key roles in various diseases, the N-terminal ATP-binding site is >85% identical, making the development of selective inhibitors challenging. In this presentation, methods used to develop isoform-selective inhibitors will be disclosed as well as some of the early preclinical studies that are being pursued for translation. Modern Aspects of Hsp90 Design and Development.



Brian S. J. Blagg

Director, Warren Family Research Center for Drug Discovery and Development University of Notre Dame, Notre Dame, IN, United States

Biography

Brian Blagg, Ph.D., Charles Huisking Professor of Chemistry and Biochemistry, is Notre Dame's first Director of the Warren Family Research Center for Drug Discovery and Development. After earning his B.A. in Chemistry and Environmental Studies at Sonoma State University, his Ph.D. in Organic Chemistry at the University of Utah, and completing an NIH Postdoctoral Fellowship from The Scripps Research Institute, Blagg started a medicinal chemistry lab at the University of Kansas in 2002. Now at Notre Dame, his lab continues its focus on the biochemical nature of chaperone proteins and protein folding in relation to cancer. Cancers are inherently more dependent on chaperone proteins because of their constant division, and Blagg's team works to selectively inhibit particular chaperone proteins to effectively halt cancer growth. His lab also studies the possibility of utilizing chaperone proteins to effectively re-fold malfunctioning proteins to treat and prevent diseases such as Alzheimer's. Blagg was attracted to Notre Dame because of the University's ambitious commitment to elevate its graduate programs. Since becoming a faculty member, he has found Notre Dame's unique atmosphere-one that includes a caring and personable administration, a strong alumni base, and a passion for knowledge-to be liberating and intellectually exciting. When not at work, Dr. Blagg enjoys watching the Irish football team and spending time with his children.

Distal functionalization via transition metal catalysis

The ubiquitous presence of sp^3 C–H bonds in natural feedstock makes them inexpensive, easily accessible, and attractive synthons for the preparation of common and/or complex molecular frameworks in biologically active natural products, pharmaceutics, agrochemicals, and materials. However, the inertness of these bonds due to the high bond dissociation energies and low polarity difference between the carbon and hydrogen atoms makes them challenging reaction partners. Moreover, the desired site-selectivity is often an issue in reactions with multiple analogous sp^3 C–H bonds. To overcome these problems, transition metal-catalyzed C–H functionalization has been developed with the assistance of various well-designed directing groups which can coordinate to a metal center to deliver it on a targeted C–H bond through an appropriate spatial arrangement, enabling C–H activation via the formation of a cyclometalated species. However, the requirement of often additional steps for the construction of the directing groups and their subsequent removal after the desired operation severely hampers the efficacy and compatibility of the reactions. A promising solution would be the utilization of a transient ligand which can bind to the substrate and coordinate to the metal center in a reversible fashion. In this way, the directing group is installed, sp^3 C–H functionalization occurs, and the directing group is then removed in situ without affecting the substrate function after the catalysis is finished. Overall, the whole process occurs in a single reaction pot. Herein, we are presenting our studies on transition metal-catalyzed transient directing group-enabled C–H functionalization reaction.

Audience Take Away Notes

- This study could potentially be used for others to build small molecules in an efficient way
- This study could potentially be used for others to carry out late-stage functionalization of natural products or drug molecules
- This research could also be used by others to expand their research



Haibo Ge

Department of Chemistry & Biochemistry, Texas Tech University, Lubbock, TX, United States

Biography

Haibo Ge received his PhD degree in Medicinal Chemistry from The University of Kansas in 2006, and then moved to The Scripps Research Institute for postdoctoral study. In 2009, he began his independent academic career at the Indiana University – Purdue University Indianapolis and relocated to Texas Tech University in 2020. Research by his group is mainly focused on the development of novel methods for carbon–carbon and carbon–heteroatom bond formation through transition metal catalyzed C–H functionalization.

Advances in plasma-based waste treatment for sustainable communities

This talk presents advanced approaches for plasma-based waste treatment. Different designs of plasma torches and generation systems are discussed, including RF, DC, and microwave plasma, are analysed and compared for waste-to-energy applications. Novel plasma torch design is proposed to support different scales of waste treatment. Process engineering techniques for gasification and pyrolysis process are illustrated with waste characterization. The proposed approaches showed reduced greenhouse gas emissions and improved lifecycle performance. Plasma systems are utilized for nuclear waste treatment for low, intermediate, and high radioactive waste. Process design is discussed for plasma torch that can reduce the volume of radioactive waste. Potential approaches are explored for mass separation that could be utilized for high-level radioactive waste. Simulation methods and experimental setups demonstrate lab-scale process technologies for plasma-based waste treatment.

Audience Take Away Notes

- Understand plasma technologies for waste treatments
- Understand ways to reduce GHG from waste treatments
- Learn practical solutions and technologies for waste treatment
- Understand ways to handle radioactive waste
- Understand potential jobs for waste management



Hossam A. Gabbar

Professor, P. Eng., Distinguished Lecturer IEEE NPSS, Director of Advanced Plasma Engineering Lab (APEL), Department of Energy and Nuclear Engineering, Faculty of Engineering and Applied Science, Ontario Tech University, Oshawa, Ontario, Canada

Biography

Dr. Hossam A. Gabbar studied systems engineering at Alexandria University. He obtained PhD degree in process systems engineering from Okayama University, Japan. He joined Japan Chemical Innovation Institute (JCCI) and Tokyo Institute of Technology. Dr. Gabbar is a full Professor in the Department of Energy and Nuclear Engineering, in the Faculty of Engineering and Applied Science, at Ontario Tech University (UOIT). He leads the Smart Energy Systems Lab (SESL), and Advanced Plasma Engineering Lab (APEL). He is the recipient of the Senior Research Excellence Aware for 2016, UOIT. He is among the top 2% of worldwide scientists in energy. He is a Distinguished Lecturer of IEEE NPSS.

Quantum theory concepts and biological evolution paths from structure waves in biopolymers

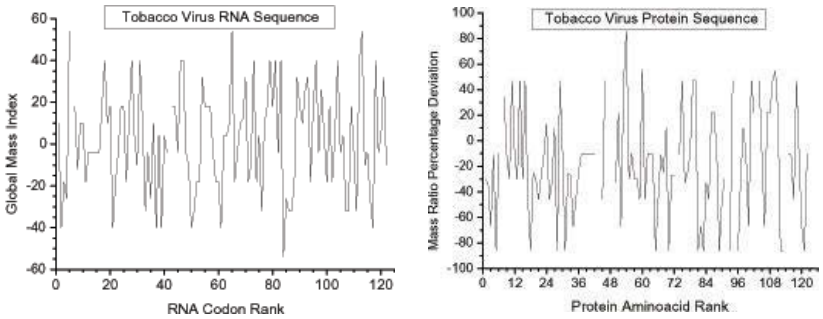
The Lamarckian theory of biological evolution assumed that changes induced by the environment on what we now call a 'phenotype' could be transferred to its 'genotype', while the Darwinian theory was based on natural and sexual selection of those 'genotypes' which showed up in fit 'phenotypes'. Darwinian mechanisms have proven quite efficient in explaining microevolution processes, but not sufficient to understand such macroevolution phenomena as speciation, radiation, and punctuated equilibria, which involve highly coordinated, structural and functional biological changes.

The fact that nucleic acids bearing the genetic material are amenable to quantum theory, as was foreseen by Schrödinger, suggests that the physico-chemical dynamics of these biomolecules and of their coded proteins over extended time scales could play a role in these coordinated changes. As wave mechanics took its roots in the de Broglie analysis of the Maupertuis and Fermat principles, one may go further and wonder if an integral formulation involving a extremum principle may not be derived for the biological evolution as well, which would make its finalist flavour compatible with the determinist views.

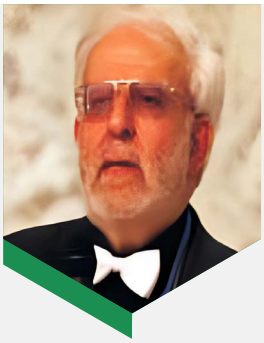
In the present talk, we propose to define a 'biological extremal principle' which could be used to uncover phylum evolution paths by maximizing the convolution of a complexity functional involving Clausius and or Kolmogorov entropies and a fitness functional to be defined from former evolution theories:

$$E[q] \equiv (G * V)[q] \equiv \iint G(q - q_a, v - v_a, t)\, V(q_a, v_a, t)\, dq_a\, dt\,; \quad \delta E / \delta q = 0.$$

As the Hamilton principle could be derived by the Feynman path-integral formulation, which involved constructive / destructive interferences of quantum waves, such an biological extremal principle may be derived from the structure waves expressing nucleic-acid and related protein structures. We propose an elaborated code for expressing such structure waves in nucleic acids and related proteins, and illustrate our code on a velvet-tobacco mottle-virus satellite RNA.



Structure waves in the RNA and derived protein of a velvet-tobacco mottle-virus satellite.



Jean Maruani

Laboratoire de Chimie Physique - Matiere et Rayonnement CNRS and Sorbonne-Universites - 7005 Paris, France

Biography

Jean Maruani was born on the 28th of December 1937 in Tunis to a middle-class Sephardic family. He makes polyvalent studies in Paris, collaborates with the CEA, the Pasteur Institute, the LCIE, and gets a Doctorat es-Sciences Physiques at Sorbonne in 1966 under the supervision of Pr Roland Lefebvre (Jury chaired by Pr Alfred Kastler). Then he takes a two-year leave to Charles McDowell's group at the Department of Chemistry of UBC (Vancouver, Canada). In 1968 he gets a permanent position at the CMOA of CNRS directed Pr Raymond Daudel. Jean Maruani has been teaching engineering students at UBC and teaching students at Sorbonne. He has published about 150 papers, mostly theoretical but also experimental, on the Structure and Dynamics of Molecular Systems, especially in Magnetic Resonance and Photoelectron Spectroscopy. He has solved a number of pending problems and introduced novel concepts for non-rigid and approximate symmetries. Later he got involved in fundamental problems related to the Dirac electron properties and also designed a quantum theory of biological evolution aimed at

reconciling determinist and finalist viewpoints. He has co-organized about 30 scientific meetings, co-edited about 50 volumes and founded a scientific journal and book series. He has created the CMOA Prize and Medal, respectively, for junior and senior scientists. Jean Maruani has a Doctorate Honoris Causa from the University of Sofia, a Golden Medal from the City of Paris, and he is Chevalier des Palmes Academiques and Corresponding Member of the European Academy. Although formally retired since 2005, he is actively involved in organizing a QSCP meeting every year in a different city of the world. He also gives talks on philosophical issues and is engaged in classical singing. In February 1969, he has married composer and pianist Marja Rantanen, from Turku (Finland): https://www.marja-rantanen.com/. They have 3 children and 6 grand-children.

Promise of herbal drugs in improving cancer radiotherapy

Cancer incidence and mortality have been rapidly increasing in the industrialized world. Discovery of new drugs for cancer treatment has been a challenging task for pharmaceutical companies. Frequently observed problems of general toxicity, exorbitant cost and non-specific action pose profound limitations in treatment of cancer patients. Among the treatment modalities, chemotherapy and radiotherapy account for more than 75 % of patient treatment. A predicament is faced in clinic because drug as well as radiation kill equally both cancer and normal cells of the patients producing undesirable side effects compelling sometimes abandoning of the treatment. Research is, therefore, needed to develop non-toxic and affordable drugs for effective treatment of patients. To meet these objectives, our laboratory has actively been investigating to develop novel drugs from plant kingdom and targeted approaches for selectively killing the cancer cells but sparing the normal cells. Apart from surgery and chemotherapy, the modality of radiotherapy is often employed mode of cancer patient treatment. While considerable improvement has been made in delivering the radiation to target diseased tissue but technical limitations yet pose many daunting challenges. A developing strategy that holds promise in treatment of cancer patients consists in searching for natural compounds with toxic properties which can selectively enhance tumor cell toxicity to radiation but spare normal cells as desired in clinical settings. Recent research from screening studies have found some potent phytodrugs from plant kingdom which display unique ability to cause no or minimal toxicity to normal cells but remarkably sensitize tumor cells to ionizing radiation. The mechanism involves the radiation generated Reactive Oxygen Species (ROS) which trigger induction of apoptosis (cellular suicide) in tumor cells because of the high oxidative stress status in these cells. This talk is designed to present a brief highlight of developing plant based herbal drugs for improving chemo and radiotherapy of cancer patients. Major part of the talk is based on the recent research results from our laboratory. A few examples of notable herbals such as Triphala, Ellagic acid and Silibinin will be given for the observed increased tumor cytotoxicity in tumor cells by certain compounds from plant sources which hold promise of improving treatment of cancer patients in radiotherapy.

Keywords: Herbal Drugs, Cancer Radiotherapy, Apoptosis, ROS, Molecular Signaling.



K. P. Mishra

Former Vice Chancellor, Nehru Gram Bharati Univ., Allahabad 211 002 India & Ex Head, RB and HS Division, Bhabha Atomic Research Center, Mumbai, India

Biography

Prof. Dr. K.P. Mishra post graduated in Chemistry from University of Allahabad. He joined prestigious National Institute, Bhabha Atomic Research Center, Mumbai as Research Scientist in nuclear Science and Technology. He grew upwards from position to position and served in the research field for more than 4 decades. He specialized in chemo-biolocal sciences, Free Radical Biology, Radiation and Cancer Biology, Biotechnology and Life Sciences. He rose to the level of Senior Professor and remained HOD for many years. He is serving on Editorial Boards of about a dozen reputed Journals. He has published more than 350 research papers in refereed reputed journals. He guided and mentored 51 Ph.D. students.

Breakthroughs and innovations in photodynamic therapy of tumors by lasers: Overview of our four decades experience

We will present an over view of our long-term team(s) experience during four decades in the field of Photodynamic Therapy (PDT) of tumors by LASER, from drug discovery to clinical applications. The lecture main topics include:

1. Our search for ideal photosensitizers and discovery of uroporphyrin ability to be selectively retained in tumors for PDT and mechanism of action.
2. We will show our novel approach of biodistribution and selective in-vivo tumor localization of endogenous porphyrins induced and stimulated by 5-Aminoleuvulinic Acid (ALA) as a newly developed technique which we adopted to treat certain types of cancers.
3. Removal of skin photo-toxicity after PDT of tumors using our novel approach.
4. We will show PDT – clinical applications for treatment of certain types of cancers.
5. Recent therapeutic application of our ALA technique in combination with high energy photons as Radiodynamic Therapy (RDT) of deep-seated tumors in lungs and brain.
6. We will present our future vision for ways to increase PDT- efficacy and where do we go from here.

Audience Take Away Notes

- Other faculty could use this research to expand their research or teaching
- This provides a practical solution to a problem that could simplify or make a designer's job more efficient
- This improves the accuracy of a design, or provide new information to assist in a design problem



Prof. Mohamed El Far

Chemistry department, Faculty of science, Mansoura University, Egypt

Biography

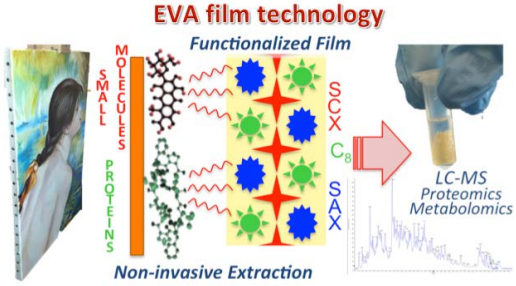
Professor El-Far published over 100 papers, received Fulbright and British council fellowships and German DAAD grant to establish PDT Program at Munich, received US-AID grant to establish PDT unit in Egypt. Serving on the editorial boards to four international journals, a visiting professor to several Universities as California, Utah laser center, Mayo clinic, Cardiff and Swansea. Selected by the IBC, Cambridge in top 100 scientists 2012. on list of global speakers for several international conferences. Selected as Mansoura university person of the year 2017/2018. Selected by Royal Swedish Academy of Science to nominate Nobel Prize winners in chemistry, year 2021.

Stroboscopic flashes on the netherworld

We describe here a modern tool for exploring documents pertaining to the world Cultural Heritage while avoiding their contamination or damage. Known under the acronym EVA, it consists of a plastic foil of Ethylene Vinyl Acetate studded with strong cation and anion resins admixed with C8 and C18 hydrophobic beads. When applied to any surface such foils can harvest any type of surface material, which is then eluted and analyzed via standard means, such as GS/MS (typically for metabolites), MS/MS (for peptide and protein analysis), X-ray (for elemental analysis). We briefly review here a number of past data, such as screening of original documents by Bulgakov, Chekov, Casanova, Kepler, while dealing in extenso with very recent data, pertaining to Orwell and Stalin and analysis of the skin of an Egyptian mummy. The technique was also successfully applied to paintings, such as the Donna Nuda at the Hermitage in St. Petersburg, attributed to Leonardo and his school. As a unique example, we quote here the analysis of a book Stalin was extensively reading during World War II (Ivan Grozny): on the pages of this book we found plenty of lithium salts, suggesting that he was bipolar just like Winston Churchill (except that this was a jealously kept secret and discovered by us for the first time as a world première). This novel methodology represents a formidable tool for exploring the past life of famous authors, scientist and literates in that it can detect traces of their pathologies and even drug consumption left by saliva and sweat traces on their original hand-written documents. Prior to our invention, the only technique proposed was scraping or grating the surface of the material under investigation, clearly a technique strictly forbidden in museums, private and public collections. In the worst cases, when dealing with pottery or other clay material, chipping away of a piece was proposed, a barbarian way to treat items belonging to the Cultural Heritage.

Keywords: Cultural Heritage, EVA Technique, Michail Bulgakov, George Orwell, Anton Chekov, Joseph Stalin, Giacomo Casanova, Johannes Kepler.

Graphical Abstract



Mixed-bed chromatographic cartridge (Expt. Rev. Proteomics 16, 2019, 533-542)
EVA: ethylene vinyl acetate film studded with strong cation and anion exchangers and with C_8 or C_{18} hydrophobic resins. It will capture any material (macromolecules and metabolites) present on the surface of items under investigation. It does NOT damage nor contaminates such surfaces.
Manfredi M, et al. Anal Chem. 2017;89:3310-3317.



Pier Giorgio Righetti[1]*, Gleb Zilberstein[2]

[1]Politecnico di Milano, Dept. of Chemistry, Italy

[2]SpringStyle Tech Design Ltd, Rehovot, Israel

Biography

Prof. Righetti earned his Ph. D. in Organic Chemistry from the University of Pavia in 1965. He then spent 3 years as a Post. Doc. at MIT and 1 year at Harvard (Cambridge, Mass, USA). He is now Emeritus Professor at the Milan's Polytechnic. He is in the Editorial Board of Electrophoresis, BioTechniques, Proteomics, Proteomics Clinical Applications. He has co-authored the books Righetti P.G., Stoyanov A., Zhukov M.: The Proteome revisited: Theory and Practice of the Relevant Electrophoretic Steps. Elsevier, Amsterdam, 2001; Hamdan M, Righetti P.G.: Proteomics Today, Wiley-VCH, Hoboken, 2005 and Boschetti E. Righetti P.G. Low-Abundance Proteome Discovery; State of the Art and Protocols, Elsevier, Amsterdam, 2013, pp. 1-341. He has developed isoelectric focusing in immobilized pH gradients, multicompartment electrolyzers with isoelectric membranes, membrane-trapped enzyme reactors, temperature-programmed capillary electrophoresis, combinatorial peptide ligand libraries for detection of the low-abundance proteome

and the EVA technique for exploration of the Cultural Heritage. On 590 articles reviewed by the ISI Web of Knowledge (Thomson Reuters) and by Mendeley Statistics, Righetti scores 31.636 citations, with an average of 47 citations/article and with a H-index of 84. During the years 2005-2013 he has received citations ranging from 1000 to 1200 per year. As a World Ranking he is No. 1161 and at a National Ranking level he is No. 23. He has won the CaSSS (California Separation Science Society) award (October 2006), and the Csaba Horvath Medal award, presented on April 15, 2008 by the Connecticut Separation Science Council (Yale University). In 2011, he has been nominated honorary member of the Spanish proteomics society and in 2012 he has won the prestigious Beckman award and medal granted in February at the Geneva MSB meeting. In 2014, in October, in Madrid, he has been given the HuPO award for proteomic research and in November, in Atlanta, the American Electrophoresis Society award.

Correlation between crystal structure, magnetic order, and topological states in $Co_3Sn_2S_2$

$Co_3Sn_2S_2$, a magnetic Weyl semimetal with a kagome lattice of cobalt ions, has triggered intense interest recently. In this talk, I will present crystal structure in both long-range and local scales, magnetism, and topological Weyl state of $Co_3Sn_2S_2$ using elastic and inelastic neutron scattering techniques. $Co_3Sn_2S_2$ was proposed to exhibit a coexistence of Ferromagnetic (FM) order and Antiferromagnetic (AFM) order below $T_C \approx 175$ K, followed by a pure Ferromagnetic (FM) order below $T_A \approx 135$ K. The long-range ferromagnetic order along the c axis was confirmed from the half-polarized neutron technology below T_C, which is correlated to the anomaly in the Co-Sn_2 bond and lattice constant a. Inelastic neutron scattering revealed highly anisotropic magnon dispersions and linewidths below T_C, and paramagnetic excitations above T_C. Modeling the spin-wave spectra shows that the ground-state FM order is dominated by the unusual third neighbor across-hexagon J_d FM coupling with a weak frustrated next-nearest-neighbor bond. Our DFT calculations reveal that the symmetry-allowed two 120° antiferromagnetic orders support new Weyl states in $T_A<T<T_C$, with distinct numbers and locations of Weyl points as compared to those observed in $T<T_A$[1].

In the second part of the talk, I will go beyond long-range scale and move to the local scale in this system. A striking local symmetry breaking from rhombohedral R-3m to monoclinic Cm co-emerges with the onset of ferromagnetic order below T_C using neutron total scattering technique. The mismatch of local and average crystallographic structures indicates that $Co_3Sn_2S_2$ becomes an intrinsically lattice disordered system below TC. This provides new insight to the previously puzzling magnetic phase separation and spin glass like state in $Co_3Sn_2S_2$. Furthermore, our DFT calculation indicates that the local symmetry breaking has the tendency to drive a local ferromagnetic moment reorientation by around 19° to the monoclinic a-axis, and plays a detrimental role in the formation of the Weyl points associated with the ground-state FM order by breaking mirror symmetries and is expected to induce a broad topological surface band like feature. Our study provides the experimental realization of dominant third neighbor cross-hexagon magnetic coupling and a hidden local symmetry breaking in a Kagome magnet, and unveils an intimate interplay between crystal structure, magnetism, and Weyl states in $Co_3Sn_2S_2$[2].

Audience Take Away Notes

- The audience could use the methodology presented in this talk on their research on magnetic materials or other functional materials. The combination of the neutron diffraction, neutron total scattering, neutron spectroscopy and DFT calculation is proved to be powerful



Qiang Zhang[1]*, Yuanpeng Zhang[1], Masaaki Matsuda[1], German D. Samolyuk[2], Matthew B Stone[1], Alexander I. Kolesnikov[1], Vasile O. Garlea[1], Rui Xue[3], David Mandrus[4,2,3], Jiaqiang Yan[2], Michael A. McGuire[2], D. Alan Tennant[2,5,6], and Satoshi Okamoto[2]

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[4]Department of Materials Science and Engineering, The University of Tennessee, Knoxville, Tennessee 37996, United States

[5]Shull Wollan Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, United States

[6]Quantum Science Center, Oak Ridge, Tennessee 37831, United States

tools to explore the interplay between crystal structure, magnetic order and topological states

- This research shows the importance to study the crystal structure in not only long-range scale but also the local scale for understanding the unusual magnetic and electronic ground states of other topological materials
- Our work indicates that the previously puzzling magnetic properties were due to an incomplete understanding of the crystalline structure of $Co_3Sn_2S_2$. It would motivate further experimental studies to discover and control local structure for realizing new structure-property relationships and engineering desired physical properties more broadly in topological semimetals and kagome magnets

Biography

Dr. Qiang Zhang is currently a staff scientist in Neutron Scattering Division, in Oak Ridge National Laboratory. Before joining ORNL, he held a position as an assistant professor at Louisiana State University. From April 2015 to March 2018, he was a research associate V in Louisiana State University and a long-term visiting scientist in ORNL. Prior to this, he was a postdoctoral research associate in Ames Laboratory & Iowa State University (2011-2015). From 2009 to 2011, he worked as a Marie Curie fellow in Laboratory CRISMAT, CNRS in France. He has published more than 150 research articles in SCI journals.

Personalized and Precision Medicine (PPM) as a unique healthcare model to be set up through biodesign-inspired, biotech-driven, chemical and bioengineering, translational applications and upgraded biomarketing to secure the human healthcare and biosafety

A new and upgraded approach to the diseased states and wellness, and to re-shape tomorrow's healthcare whilst doing it today, resulted in a new global trend in the healthcare services, namely, Personalized and Precision Medicine (PPM). PPM as a Unique Entity demonstrating an integration of Fundamental, Healthcare & Life Sciences, Biodesign-driven BioTech, Translational ART and IT Armamentarium, is based on the new developmental strategy driven by Biomarkers- and Biotargeting-related biomachines. So, it would be extremely useful to integrate data harvesting from different databanks for applications such as pre-early predictive diagnostics, precise prognostication and personalization of further treatment to thus provide more tailored measures for the diseases bodies and persons-at-risk resulting in improved outcomes and more cost effective use of the latest health care resources.

PPM as being the Grand Challenge to forecast, to predict and to prevent is rooted in a big and a new SCIENCE generated by the achievements of (i) Systems & Synthetic Biology; (ii) Biodesign-driven Translational applications and Biotech-driven Biomanufacturing; (iii) Bioindustry and Biomarketing of the next step generation. The latter, being a Grand Brick laid into the frame of National Bioeconomy, says and confirms that the efficiency and efficacy of the Bioeconomy are determined and dictated by the innovative trends, generated by fresh knowledge and their transfer into the scientific, bioindustrial and social areas to maintain the national stability and extensive development of the country.

The core strategic tool to operate the transdisciplinary approach is rooted in a unique tandem consisting of (i) integrated platforms of Fundamental Sciences (Basics) and innovative OMICs biotechnologies on one hand, and (ii) the algorithms of Bioinformatics, on the other one.

Healthcare is undergoing a transformation, and it is imperative to leverage new technologies to support the advent of PPM. This is the reason for developing global scientific, clinical, social, and educational projects in the area of PPM and TraMed to elicit the content of the new trend. The latter would provide a unique platform for dialogue and collaboration among thought leaders and stakeholders in government, academia, industry, foundations, and disease and patient advocacy with an interest in improving the system of healthcare delivery on one hand and drug discovery, development, and translation, on the other one, whilst educating the policy community about issues where biomedical science and policy intersect



Sergey Suchkov[1-6]*, Daniel Scherman[9], Shawn Murphy[7,8], David Smith[10], Hiroyuki Abe[5], Holland Cheng[11], Noel Rose[7,8,12]

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[2]A.I. Evdokimov MGMSU, Moscow, Russia

[3]EPMA, Brussels, European

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[5]ISPM, Tokyo, Japan

[6]AHA, Houston, TX, United States

[7]MGH, United States

[8]Harvard Medical School, Boston, MA, United States

[9]Centre de Recherche Pharmaceutique de Paris (CRP2); Faculte de Pharmacie, Universite Paris Descarte, Centre National de la Recherche Scientifique, Unite de Technologies Chimiques et Biologiques pour la Sante (UTCBS) Inserm, Paris, France

[10]Mayo Clinic, Rochester, MN, United States

[11]T College of Biological Sciences, UC Davis, CA, United States

[12]Center for Autoimmune Disease Research, John Hopkins University, Baltimore, MD, United States

Audience Take Away Notes

- Only positions and vacancies of the next step generation including practitioners passed through PPM-guided clinical residency
- For teaching clinical practice in Personalized and Precision Healthcare Services (PPHCS), including PPHCS-driven cardiology, nephrology, oncology, hematology, neurology and gastroenterology
- Directly. PPM would depict approaches aiming at the development of PPM-driven biodesign-inspired translational research and applications
- It 100% improves the accuracy of a design, or provide new information to assist in a design problem

Biography

Sergey Suchkov was born in the City of Astrakhan, Russia, in a family of dynasty medical doctors. In 1980, graduated from Astrakhan State Medical University and was awarded with MD. In 1985, Suchkov maintained his PhD as a PhD student of the I.M. Sechenov Moscow Medical Academy and Institute of Medical Enzymology. In 2001, Suchkov maintained his Doctor Degree at the National Institute of Immunology, Russia. From 1989 through 1995, Dr. Suchkov was being a Head of the Lab of Clinical Immunology, Helmholtz Eye Research Institute in Moscow. From 1995 through 2004 - a Chair of the Dept for Clinical Immunology, Moscow Clinical Research Institute (MONIKI). In 1993-1996, Dr. Suchkov was a Secretary-in-Chief of the Editorial Board, Biomedical Science, an international journal published jointly by the USSR Academy of Sciences and the Royal Society of Chemistry, UK. At present, Dr. Sergey Suchkov, MD, PhD, is Professor and Chair, Dept for Personalized Medicine, Precision Nutriciology and Biodesign, the Institute for Biotech & Global Medicine of RosBioTech, Moscow, Russia. Professor, Dept for Clinical Immunology, A.I. Evdokimov Moscow State University of Medical and Dentistry, Moscow, Russia. Member, New York Academy of Sciences, USA. Secretary General, United Cultural Convention (UCC), Cambridge, UK. Dr. Suchkov is a member of the American Chemical Society (ACS), USA; American Heart Association (AHA), USA; European Association for Medical Education (AMEE), Dundee, UK; EPMA (European Association for Predictive, Preventive and Personalized Medicine), Brussels, EU; ARVO (American Association for Research in Vision and Ophthalmology); ISER (International Society for Eye Research); Personalized Medicine Coalition (PMC), Washington, DC, USA.

Co_2-assisted dehydrogenation of propane to propene over Zn-BEA zeolites: Impact of acid–base characteristics on catalytic performance

Research results about the influence of BEA zeolite preliminary dealumination on the acid–base characteristics and catalytic performance of 1% Zn-BEA compositions in propane dehydrogenation with CO_2 are presented. The catalyst samples, prepared through a two-step post-synthesis procedure involving partial or complete dealumination of the BEA specimen followed by the introduction of Zn^{2+} cations into the T-positions of the zeolite framework, were characterized using XRD, XPS, MAS NMR, SEM/EDS, low-temperature N_2 ad/desorption, C_3H_8/C_3H_6 (CO_2, NH_3)-TPD, TPO-O_2, and FTIR-Py techniques. Full dealumination resulted in the development of a mesoporous structure and specific surface area (BET) with a twofold decrease in the total acidity and basicity of Zn-BEA, and the formation of Lewis acid sites and basic sites of predominantly medium strength, as well as the removal of Brønsted acid sites from the surface. In the presence of the ZnSiBEA catalyst, which had the lowest total acidity and basicity, the obtained selectivity of 86–94% and yield of 30–33% for propene (at 923 K) exceeded the values for ZnAlSiBEA and ZnAlBEA. The results of propane dehydrogenation with/without carbon dioxide showed the advantages of producing the target olefin in the presence of CO_2 using Zn-BEA catalysts.

Audience Take Away Notes

- The audience will be able to understand as control of preparation of catalyst systems
- They will see that catalytic activity depend on dispersion of metal in the framework of zeolite
- The researchers will be able, after my talk, do their own catalyst preparation using similar method



Stanislaw Dzwigaj

Sorbonne Universite, UMR 7197, Laboratoire de Reactivite de Surface, France

Biography

Professor Stanislaw Dzwigaj received his PhD degree in 1982 in Jerzy Haber Institute of Catalysis and Surface Chemistry, Krakow (Poland). After two years of postdoctoral stay at the Laboratoire de Reactivite de Surface Universite P. et M. Curie (Paris) he obtained in 1990 a position of contracted researcher in the same Laboratory devoted to surface reactivity in relation to catalysis phenomena. Then, in 2008 he obtained permanent position in CNRS as a researcher. On February 19, 2014 for outstanding scientific achievements, he received the title of professor. His published work includes more than 180 papers published in reputable international journals.

Novel therapeutics for common and devastating chronic obstructive pulmonary disease

As the third leading cause of mortality in the world, Chronic Obstructive Pulmonary Disease (COPD) is a common and devastating lung disease. However, the current clinical therapeutic options for COPD are limited, and its molecular mechanisms remain largely unknown. COPD is well characterized by airway hyperresponsiveness and remodeling, thereby leading to airflow limitation. We and other well-known scientist have unveiled that a Very Important Player (VIP) in airway hyperresponsiveness and remodeling of COPD is an increase in intracellular calcium ($[Ca^{2+}]_i$) in Airway Smooth Muscle Cells (AMCs). Consistent with this view, bronchodilators including muscarinic receptor antagonists, β-adrenergic receptor agonists and corticosteroids are used as the first-line drugs in the clinical treatment of COPD, and the functional role of all these forefront drugs are associated with their inhibition of the increased $[Ca^{2+}]_i$ in ASMCs. Recent studies from our group and others suggest that multiple ion channels, particularly Inositol Trisphosphate Receptor (IP_3R)/Ca^{2+} release channel, Ryanodine Receptor (RyR)/Ca^{2+} release channel and canonical Transient Receptor Potential-3 (TRPC3) channel, play a major role in initiation and maintenance of $[Ca^{2+}]_i$ in ASMCs and thus are essential for airway hyperresponsiveness and remodeling in COPD and/or other pulmonary diseases. Equally interestingly, IP_3R, RyR and TRPC3 channels are highly sensitive to Reactive Oxygen Species (ROS), and ROS are well known to mediate airway hyperresponsiveness and/or remodeling in COPD. We have further reveal that ROS are primarily produced by mitochondria and NADPH oxidase (NOX), but mitochondria are the primary site. Several antioxidants targeted at mitochondria and/or NOX are currently used in clinical trials and show potential effectiveness in the treatment of COPD. ROS may implement their roles in COPD by causing oxidation of IP_3R, RyR and TRPC3 channels, leading to their hyperfunctions. We and other eminent investigators have further provided new evidence that virus-mediated shRNA-based genetic (specific) inhibition and highly selective pharmacological inhibitor of these channels may become more effective therapies for COPD.

Audience Take Away Notes

- My current presentation will greatly help the audience to create their future research directions
- The finding presented may significantly assist the audience to develop novel preventive and therapeutic strategies for COPD and other relevant pulmonary diseases
- Our research could also be used by other investigators to expand their research and/or teaching
- All my presentation may also greatly improve experimental design, implementation, data analysis, explanations, statements, and/or conclusions



Yong-Xiao Wang, MD, PhD

Department of Molecular & Cellular Physiology Albany Medical College Albany, New York, United States

Biography

Dr. Wang has been a Full Professor in at Albany Medical College since 2006. He had his MD at Wannan Medical University in 1983, PhD at Fourth Military Medical University in 1990, postdoctoral training at Technology University of Munich in 1993 and University of Pennsylvania in 1995, and Assistant Professor (research) at University of Pennsylvania in 1997. Dr. Wang has had numerous publications in Nature Commun (impact factor: 17.694), Antioxid Redox Signal (8.401), Proc Natl Acad Sci USA (12.779), Nature (69.504), Circ Res (23.218), and other highly peer-reviewed journals and served as the editorial board member, section editor, and the executive committee member and/or subcommittee chair.

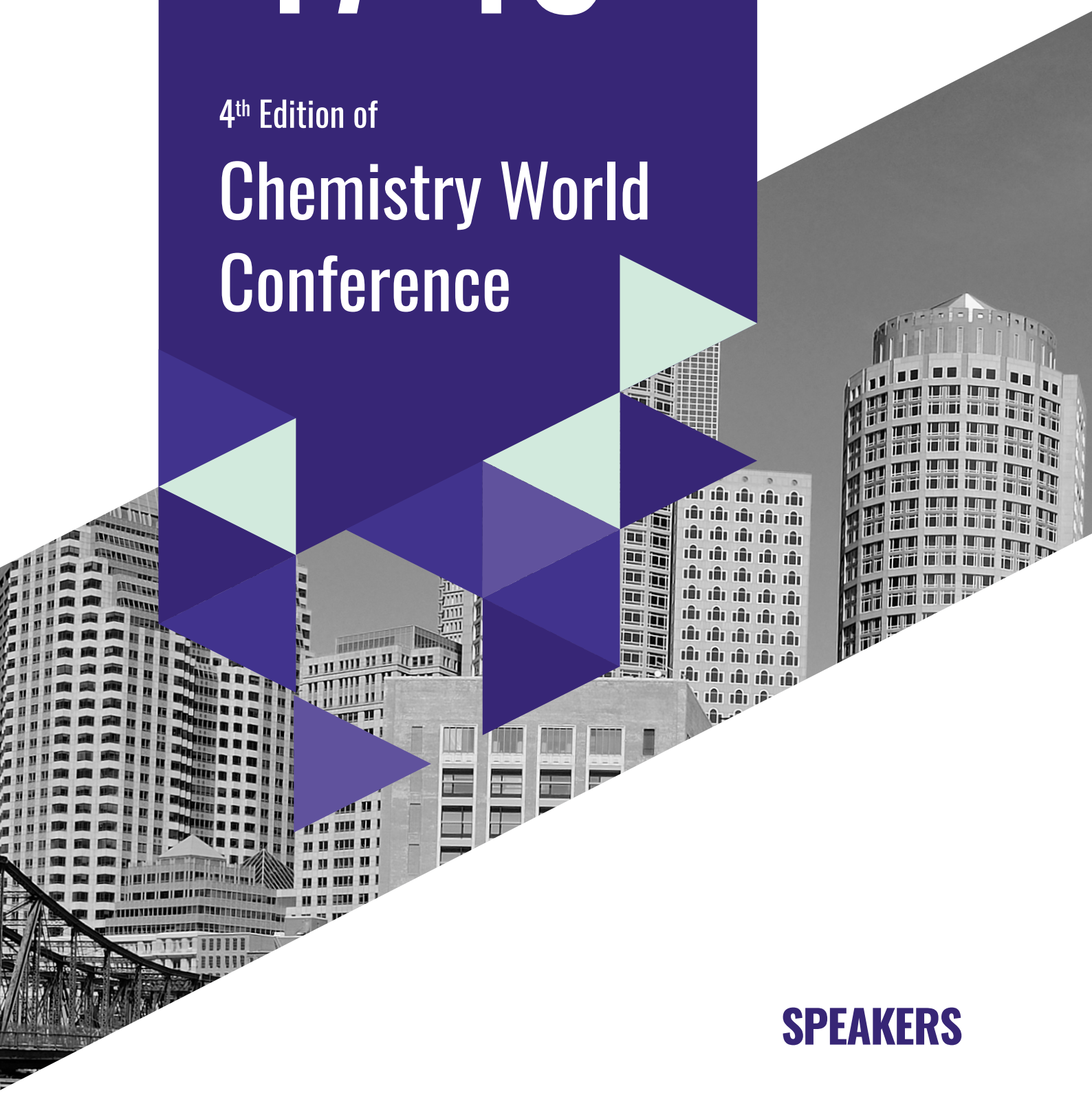
BOOK OF ABSTRACTS

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Chemistry World Conference



SPEAKERS



Andre Dias[1], Pedro Dias[1], Mohammed Mamor[2], Abel Rouboa[1]*

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Syngas and power generation from date palm waste steam gasification

This study uses the aspen plus program to simulate the gasification process of biomass conversion into energy. Aspen Plus is an extremely potent simulation tool that was utilized in this instance to assess the feasibility of utilizing a particular waste as biomass and forecast the outcomes of integration in a power generation system.

Date palm waste was selected as the feedstock to be used as the main source of energy (DPW). The Middle East has an abundance of it. The two components of this effort are the creation of syngas from date palm trash through steam gasification and the production of electricity from the syngas. Using the assumption that the material had been dried, the literature provided the physical and chemical analysis of DPW. Based on Gibb's free energy minimization, all processes were shown to have reached thermodynamic equilibrium. Steam is preferable for enriching hydrogen because it increases the water gas shift process; nonetheless, it is more expensive than air for this study work's gasification. The model primarily comprises of a gasifier that uses steam to gasify waste paper and produce hydrogen-rich syngas. Following compression, it is burned in a combustion chamber and fed into a gas turbine to produce energy. In order to heat input water, create steam, and subsequently provide power for the turbine, the system also has a steam turbine that recovers waste heat from processes in the gasifier and gas turbine. Upon acquiring the model, multiple analyses were conducted to acquire the desired outcomes. The effects of the steam/biomass ratio and the gasification temperature on the volume composition and LHV were investigated in order to assess the quality of syngas.

According to the data, H_2 contributes the most molarity (37%). The temperature at which gasification occurs causes a modest drop in H_2 content, a rise in CO content, and a decrease in CO_2. Between 650°C and 900°C, the resulting syngas's LHV ranged between 5,55 MJ/m3 and 5,65 MJ/m3. The data also demonstrate that the H_2, CO_2, and CO contents, together with the LHV, decrease with an increase in the steam/biomass ratio. In terms of power generation, a feedstock of 1000 kg/h of DPW produced about 2,3 MW using the simulation settings selected. Eighty-three percent of this power was created by the gas turbine, with the remaining power coming from the steam turbine using the recovered heat. The impact of various factors, including the air flowrate, compression ratio, and steam/biomass ratio, on the final product was also investigated. The findings show that as the steam/biomass ratio rises, more power is produced because of the increased flowrate of the combusted gases and the increased compression ratio. Ultimately, it was found that larger air flowrates result in richer combustion and higher mass flowrates of the gas products, both of which increase power output. Following a very basic economic analysis, the cost of producing one kWh of electricity was 0,0969 €.

Biography

Dr. Rouboa studied Mechanical Engineering at the University of Pierre et Marie Curie, Paris, France, and graduated as MS. He then joined the research group of CEA (Centre d'Energie Atomique at Saclay). He received his PhD degree in 1994 at the same university with CEA Laboratories. After one year postdoctoral fellowship supervised by Prof. Rene Gibert at the LIMSI Laboratory, CEA (Saclay, France), he obtained the position of Assistant Professor at University of Paris

VI, then University of UTAD from 1999 to 2021 as Assistant and Associate Professor and then Faculty of Engineering of University of Porto from September 2021 until now as Tenure Associate Professor. He supervised 11 concluded PhD thesis and supervising 3 other PhD thesis in Energy Conversion field. He has published more than 120 research articles in SCI(E) journals.), he has 40 as Hirsch Index (Scopus) and 48 (Google Scholar) and has been cited 5723 times (Google Scholar).



Asiful H. Seikh[1]*, Jabair A. Mohammed[1], Ubair A. Samad[1], Mohammad A. Alam[1], Saeed M. Al Zahrani[2], El Sayed M. Sherif[1]

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[2]Department of Chemical Engineering, College of Engineering, King Saud University, P.O. Box—800, Riyadh 11421, Saudi Arabia

Effect of Micaceous Iron Oxide(MIO) and nano crystalline Al on the electrochemical behavior of aliphatic amine cured epoxy coating

Three coating formulations were fabricated by incorporating different percentages of MIO (1, 2 and wt%) with ball milled nano crystalline Al (2 wt%) particles which was optimized earlier. These coatings were characterized by means of different methods; namely, SEM, TGA, pendulum hardness, scratch test, and nano-indentation. The EIS measurements were carried out to report the effect of adding MIO powder in fabricated coatings on their corrosion behavior in 3.5 wt% NaCl solutions. In order to report the effect of immersion time on the corrosion and degradation of the prepared coatings, the EIS data were also acquired after various exposure periods of time, i.e. 1 h, 7 d, 14 d, 21 d, and 30 d in the test chloride solution. It has been found that the obtained EIS data for the fabricated coatings proved that the presence of 2% MIO provided the highest corrosion resistance amongst all coatings and that effect was recorded after all immersion periods of time. But the MIO incorporated coatings has less corrosion resistance than Al based epoxy coatings. It was also shown that with prolonged immersion the resistance to corrosion declined after 7d then with longer period of immersion i.e 14 d, 21 d, and 30 d increases the resistance to corrosion by forming oxide products on the coatings surface. The results obtained from both mechanical and electrochemical testing confirmed that the fabricated coating with 2 wt% Al exhibited better hardness and higher resistance to corrosion as compared to coatings with 1 wt% Al and 3 wt% Al.

Audience Take Away Notes

- The audience can understand the corrosion resistance can be enhanced with the nanocrystalline materials
- The coating companies can use the nano pigments to protect structures
- The faculties can understand the processing of nano pigmented coatings and mechanism of corrosion resistance
- This provides a practical solution to a problem that could simplify or make a designer's job more efficient
- It improves the accuracy of a design, or provide new information to assist in a design problem
- Mechanical and electrochemical corrosion resistance properties increase

Biography

Dr. Seikh has completed his PhD in Materials and Metallurgical Engineering from Jadavpur University, India. He is the Associate Professor of King Saud University, KSA. He has over 100 publications that have been cited over 1000 times, and his publication H-index is 20 and has been serving as an editorial board member of reputed Journals.



Amr Awad Ibrahim, Doaa A. Kospa, Salma M. Abo Kamar, Ahmed A. Salah, S. A. El Hakam, Awad I. Ahmed*

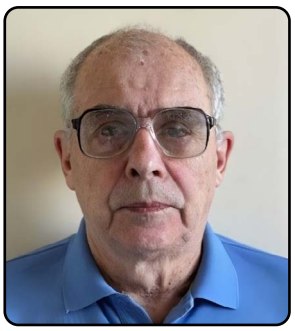
Department of Chemistry, Faculty of Science, Mansoura University, Al-Mansoura 35516, Egypt

The role of reduce graphene oxide content on the adsorption-enhanced photocatalysis and antibacterial activity of reduced graphene oxide/ bismuth tungstate nanocomposites

One of the main health issues of modern times is the lack of access to clean drinking water. Industrial dyes are among the most prevalent substances that make water dangerous to drink. Among these dyes, Methylene Blue (MB) and Rhodamine B (RhB) are the most dangerous for both the natural environment and human health. Semiconducting-based heterogeneous photocatalysis generates high redox power charge carriers under solar illumination, making it a successful approach for cleaning wastewater from pollutants. Consequently, nanocomposite catalysts have a stronger capacity to catch light, strong redox capabilities, and a range of oxidation and reduction sites. The current work uses a simple solvothermal approach to generate a novel nanocomposite photocatalyst, rGO/Bi_2WO_6. Many analytical and spectroscopic approaches involving powder X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDS), Photoluminescence (PL), X-ray Photoelectron Spectrometer (XPS}, Fourier-Transform Infrared Spectroscopy (FT-IR), Transmission Electron Microscopy (TEM), and UV-vis Diffuse Reflectance Spectroscopy (DRS) were used to characterize the synthesized solar light-driven nanocomposites. The oxidation of MB and Rh B dyes in the presence of solar light was used to assess the photocatalytic efficiency of the rGO/ Bi_2WO_6 combination. In addition, the effects of catalyst loading, starting substrate concentration, rGO content, and reaction pH were investigated. The photocatalytic activity of the generated catalyst was also compared to that of bare Bi_2WO_6 under ideal conditions. Under visible light irradiation, the addition of rGO increases the degradation efficiency of MB and Rh B, with the most favorable findings obtained with 10rGBi_2WO_6 calcined at 250 °C. After 30 minutes of exposure, the synthesized nanocomposites in the visible area showed good photodegradation percentages of 100.0% and 87.6% for MB and RhB dyes, respectively. Furthermore, the higher photocurrent responsive intensity and lower arc radius of electrochemical impedance of rGO/Bi_2WO_6 compared to Bi_2WO_6 revealed a synergistic effect on Bi_2WO_6 visible light responsiveness. Electrochemical Impedance Spectroscopy (EIS) and Cyclovoltammetry (CV) were used to evaluate the electrochemical characteristics of the synthesized materials. According to the findings, rGO/Bi_2WO_6 has the lowest charge-transfer resistance and the largest specific capacitance. The improved photocatalytic activity of rGO/Bi_2WO_6 is due to the synergistic action between rGO and Bi_2WO_6 that induces the separation of photo-generated charge carriers. Based on these observations, a viable degradation pathway for MB and RhB dyes was proposed. 10rGBi_2WO_6 demonstrated excellent charge separation, stability, reusability, and photocatalytic activity. Furthermore, the antibacterial efficacy of gram-positive Bacillus subtilis and gram-negative Escherichia coli bacteria was found to be around 96.5% and 86.3%, with corresponding zones of inhibition measuring 21 and 19 mm, respectively.

Biography

Awad Ibrahim Ahmed, is a professor of Physical Chemistry at the Faculty of Science, Mansoura University. Dr Ahmed earned his B.SC in 1974 from Mansoura University and MS.C in 1978. In 1981 Dr. Awad earned his Ph.D. in Physical Chemistry (Surface and Catalysis), also In 2024 Dr. Ahmed earned a D.SC in Physical Chemistry. In 2008, Dr. Ahmed was assigned as Head of the Chemistry department at the Faculty of Science at Mansoura University till 2010. Also, he was selected as a Member of the Faculty of Science Council from 2018 till now. In 2014 Dr Ahmed was assigned as a Program Director for the Petrochemical Program at the Faculty of Science at Mansoura University. He is currently leading his research group (50 graduate students) in material science and its applications such as Energy, Catalysis, and Seawater desalination. Dr. Ahmed received several funded projects from Science and Technology& Innovation Funding Authority (STDF), National Academy of science and Mansoura University research unit (around 10 million Egyptian pounds) in the field of Li-ion batteries, water Desalination, and supercapacitors. He published more than 75 papers in highly prestigious journals. Awad has received many awards including Mansoura University Research Excellence Award in 2023.



Stul' Boris Ya
Research institute Sintez, Moscow, Russian Federation

Kinetics of the oxyethylation reaction of alcohol taking into account the influence of association. Apparent rate constants in the liquid phase chemical kinetics

The reaction of oxyethylation of alcohols can be represented by the following scheme

$$ROH \xrightarrow[k_0,obs.]{C_2H_4O} ROC_2H_4OH \xrightarrow[k_1,obs.]{C_2H_4O} RO(C_2H_4O)_2H \xrightarrow[k_2,obs.]{C_2H_4O} \text{etc}$$

This is an irreversible alcohol-sequential reaction that can have many stages, but in this case we are mainly talking about the first stage of the reaction, characterized by the rate constant $k_{o, obs}$.

Primary alcohols of normal structure C_1–C_7 and C_{10} were studied. The reaction was carried out at t = 80-180°C and P = 1.5 MPa.

Studies have shown that the reaction rate in almost all cases is of the first order in the concentration of alcohol associates. This occurs, apparently, because the reaction product remains in the associate as a terminal molecule and, having a lower reactivity, does not allow it to participate in a further reaction.

The exception is methanol. At 80 and 100 °C, the reaction rate is of the first order in alcohol concentration. This occurs because the reaction product leaves the associate. This can be explained by the fact that methanol, under these conditions, apparently exists in the form of comb-shaped associates with a coordination number close to 3, whereas other alcohols exist under these conditions in the form of linear chain associates with a coordination number close to 2. Although methanol reacts as an associate, the resulting rate constant automatically refers by default to the monomeric alcohol molecule.

In modern liquid-phase chemical kinetics, first-order reactions are very common. This is due to the fact that although an associate almost always enters into a reaction, almost as often the reaction product leaves the associate. First order in the concentration of the associated reactant is observed and the default rate constant automatically refers to the monomeric molecule of the associated reactant. The differences can be quite significant. For example, an ethanol molecule in a state close to monomeric (n≈1, solvent dodecane) at 100 °C has a rate constant for the oxyethylation reaction $k_{o, obs}$. $=1\times10^{-3}L^2/mol^2 \cdot s$. In almost pure alcohol (n=25.7) $k_{o, obs}$. $=11.4\times10^{-3}L^2/mol^2 \cdot s$. That is, the ratio of rate constants calculated based on the alcohol concentration will be equal to 11.4. If the calculation is carried out based on the concentrations of associates, then the ratio will be another 25.7 times greater, that is, it will be equal to 290.

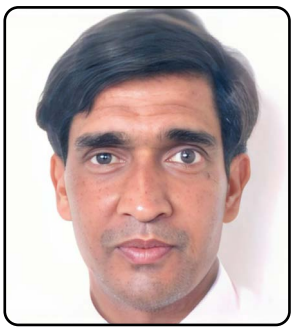
Thus, in liquid-phase chemical kinetics, the first-order rate constants with respect to the associated component are apparent. They do not reflect the actual reactivity of monomeric molecules. Ideally, the parameters of the associate to which this constant refers should be specified.

Audience Take Away Notes:

- It is advisable for university teachers of chemical kinetics courses to familiarize themselves with the work

Biography

Stul' Boris Ya. Graduated from the Department of Physical Chemistry of the Russian State University of Oil and Gas named after.I.M. Gubkin. He is author of ~80 scientific papers. Currently he engaged in the chlorination and ethoxylation of organic compounds.



Brij Bhushan Tewari
Department of Chemistry, Faculty of Natural Sciences, University of Guyana, Georgetown, Guyana

Phytochemical analysis, antifungal and antibacterial screening of Artocarpus altilis: Guyana flora extracts

The plant material leaves of Artocarpus altilis (Breadfruit) were collected from university of Guyana road, Cummings lodge, Guyana. Leaves are dried in oven at 50-55 °C for 72 h. The moisture content is calculated. The dried leaves were grounded and extracted in each acetone, ethanol and methanol solvents. Extracts were collected and evaporation of solvent was done on rotavapour. The respective solvent was added to viscous semi solid liquid extract to make up the desired volume of extract solution. The antimicrobial and antifungal activity of both plants were examined by well diffusion method, poison plate method, paper disc plate method and streak plate methods. In Artocarpus altilis leaves extract studies, maximum and minimum antimicrobial potential was observed for methanol and acetone solvent extracts, respectively. All plant extracts showed antimicrobial potential toward the organisms Staphylococcus aureus, Escherichia coli and Candida albicans. The phytochemical analysis of methanol leaves extract of breadfruit tested positive for flavonoids, terpinoids, phenol, phlobatannins, steroids and phytosteroids and negative for tannins, saponins, alkaloids and cardiac glycosides. It is observed from the present studies that leaves extract of Artocarpus altilis have antimicrobial property and its potential increases as their amount increases. Medical benefits of breadfruit extracts include, cardiovascular health, good for skin, reduce diabetes, dental health, energy booster, bone health, sleep better at night, resistance against infection etc. The wood of breadfruits one of the most valuable timbers in the construction of traditional houses. Breadfruit contains phytochemicals having potential as an insect repellent. Present research work is very useful for the researchers of similar research interest.

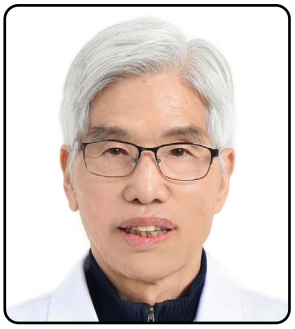
Audience Take Away Notes

- Audience can initiate to study in the same research area
- Audience can expand their research work of similar research interest
- Audience can study Medical applications of more local medicinal plants
- The knowledge gained can be used to enhance their teaching and research
- Audience can teach medical applications of green drugs
- Audience can also teach their students about medicinal potentials of natural products
- Any faculty member can use present work in their teaching and research
- Medical potential of local green drugs can be studied
- Phytochemical screening of local medicinal plant can be attempted
- Present study can be modified in following ways to make it more efficient
- Using more polar solvents for the extraction of plant parts
- Using more plant and human pathogens for the study
- Study more phytochemicals
- It improves the accuracy of a design, or provide new information to assist in a design problem

- Accuracy of result can be improved by accurate measurement of inhibitory zone
- Triplicate experiment
- Phytochemical screening can be done by two methods
- Other benefits
    - Studies on medical potential of local medicinal plants can be attempted
    - Crude green drugs can be prepared and tested
    - Further studies on more phytochemicals can be attempted

Biography

Dr. Brij Bhushan Tewari is a Professor in Chemistry in the Department of Chemistry at University of Guyana. Prof. Tewari obtained the Doctor of Philosophy (D. Phil) degree in Science (Chemistry) 1985 from Allahabad University, India and Doctor of Medicine (MD) from Texila American University. He has taken teaching/research appointments at several universities in Asia, Europe, USA, Canada and Guyana. His major research interests are in the area of (i) Metal complexes in biology and medicine (ii) Astrobiology & chemical evolution and origins of life (iii) Environment, Microbiology and Agriculture. He has published 138 research papers in international journal, one book and nine book chapters.



Dae Dong Sung[1]*, Kim Gyu Ah[1], Youngjin Lee[2], Duckjoo Lee[3]

[1]Department of Advanced Materials Chemistry, Korea University, Samse Medical Center, Sejong-si, Korea

[2]Department of Medicine, Cha University, AEM Bio Integrative Medicine Center, Seoul, Korea

[3]GC Cell Corporation, GC group, Seoul, Korea

The role of chemistry in contribution to biomedicine recently

Recently, chemistry has made a significant contribution to the field of biomedicine.

Among the areas of biomedicine, chemistry is making a significant contribution to the anti-aging field, which aims to realize the dream of gene scissor therapy and life extension.

Measurements of analysis of cellular heterogeneity in gene expression are available by using a variant of flow cytometry based on fluorescence or light scattering to sort cells. This tool is based on molecular spectroscopy. Laser capture microdissection is helpful to identification that is coupled to a microscope and focused on a tissue.

Molecular mass spectrometry is contributed to RNA sequencing tool based on headspace solid-phase microextraction/gas chromatography-mass spectrometry.

Inflammation is one of the major causes of cellular senescence. Inflammatory aging is characterized by increased levels in the proinflammatory factors in the cells. The cell changes lead to the aging of the cells. Senescent fibroblasts and keratinocytes secrete a large number of senescent associated secretory phenotypes including the pro-inflammatory cytokines induce cell senescence by promoting the production of ROS and activating the ATM /p53/p21-signaling pathway.

Fibroblasts positive for SA-beta-gal activity and p16 expression are available to reveal immunofluorescent imaging to be identified the senescent fibroblasts.

Utilizing quantum theory in the field of biomedicine can help in understanding and applying treatments for a multitude of different disease or diverse types of cancer, and even expand upon efficient and reliable diagnosis in clinical settings.

Quantum chemistry gives an important explanation for subtle DNA changes and even telomere shortening in cancer patients. Using quantum chemistry in the field of biomedicine is available to understand and to apply treatments for multitude of different disease as Alzheimer's disease and divers types of cancer, and to expand on efficient and reliable diagnosis in clinical treatments.

Computational chemistry's tool is contributed to improve biomedicine drug development as molecular dynamics simulations and density functional theory. More recently, artificial intelligence connected to computational chemistry is largely contributed.

Quantum chemistry can provide valuable insights and a different perspective regarding the interaction between receptor and ligand in structure-based drug design, the holy grail of computational biomedicine drug discovery.

Biography

Professor Dae Dong Sung studied chemistry at Dong-A University as BS and MS in 1979 and Princeton University as Ph.D. 1982. He joined the research group of Professor Donald Bethel at Liverpool University as the Royal Society Fellow of Chemistry UK. He joined the research group of Professor Hideo Tomioka at Mie University Japan as visiting Professor. He studied very fast intermediate molecules in the field of physical organic chemistry. He worked Professor After completing his degree, he worked at Dong-A University and Korea University as professor of physical organic chemistry. He has published more than 240 research articles in SCI journals.



Emil Kartalov
Naval Postgraduate School, US Dept of the Navy, USA

A solution to the clearance problem of sacrificial material in 3D printing of microfluidic devices

3D-printing is poised to enable remarkable advances in a variety of fields, such as artificial muscles, prosthetics, biomedical diagnostics, biofuel cells, flexible electronics, and military logistics. The advantages of automated monolithic fabrication are particularly attractive for complex embedded microfluidics in a wide range of applications. However, before this promise can be fulfilled, the basic problem of removal of sacrificial material from embedded microchannels must be solved. The presented work is an experimental proof of principle of a novel technique for clearance of sacrificial material from embedded microchannels in 3D-printed microfluidics. The technique demonstrates consistent performance (~40–75% clearance) in microchannels with printed width of ~200 μm and above. The presented technique is thus an important enabling tool in achieving the promise of 3D printing in microfluidics and its wide range of applications.

Audience Take Away Notes:

- Expand understanding of 3D printed microfluidics, its challenges and applications
- Learn about new capabilities applicable in multiple fields
- The presented research is relevant in both teaching and subsequent research
- The presented research contains a practical solution to a tough problem
- Presented solution has far reaching consequence to microfluidic design and engineering

Biography

Dr. Emil Kartalov holds a B.S. in Physics, M.S. in Applied Physics, and Ph.D. in Applied Physics, all from California Institute of Technology. In 2004, Dr. Kartalov joined the University of Southern California (USC) as a postdoctoral scholar. In 2006, he won a K99/R00 career award from NIH and became faculty at USC in 2008. In 2016, Dr. Kartalov moved to the Naval Postgraduate School to take his current position as Associate Professor of Physics. Dr. Kartalov has 32 issued US patents and 33 peer-reviewed publications.



Eva Falomir*, Alberto Pla Lopez

Inorganic Chemistry Department, Jaume I University, Avda. Sos Baynat SN, 12071 Castellon, Spain

Aryl azole derivatives as potential disruptors of tumor microenvironment

Thirty-nine aryl azoles, were synthesised and biologically evaluated for their activity as tumour microenvironment disruptors. Antiproliferative studies were performed in the tumour cell lines HT-29, A- 549 and MCF-7 and in the non-tumour cell line HEK-293. In HT-29, expression levels of biological targets involved in tumour microenvironment processes such as PD-L1, CD-47, c-Myc and VEGFR-2 were assessed. In addition, the antiproliferative activity was assessed when HT-29 were co-cultured with THP-1 monocytes and the secretion levels of IL-6 were also determined in these co-cultures. The angiogenic effect of some selected compounds on HMEC-1 was also evaluated as well as their effect on vasculogenic mimicry on HEK-293. Compounds with an amino group in the phenyl ring and a halogen atom in the benzyl ring showed promising results as tumour microenvironment disrupting agents. The most outstanding compound dramatically reduced the population of HT-29 cells when co-cultured with THP-1 monocytes and the levels of IL-6 secreted, as well as showing moderate effects on PD-L1, CD-47 and c-Myc.

Audience Take Away Notes

- Those people in the audience involved in Drug Discovery research could use most of the information we are going to provide
- This is a multidisciplinary and interdisciplinary work so people from research fields involved in Medicinal Chemistry, Biochemistry, Organic Chemistry, Cell biology, Immunology could be interested
- The audience will learn more about multitarget anticancer drug discovery for oncoimmunomodulating therapies

Biography

Dr. Eva Falomir received her PhD degree in 1998 at Jaume I University (Spain). After two years postdoctoral fellowship supervised by Dr. A. Furstner at Max-Planck Institute, Germany she obtained the position of an Associate Professor at UJI. In 2022, she got a Full Professor position in the same university. She has published more than 100 research articles in SCI(E) journals. In the last 10 years, she has become the leader of her own research group which is focused on the design, synthesis and biological evaluation of new small molecules with anticancer, antiangiogenic and immunomodulatory activity.



Farshad Akbarnejad
Scientific Department, Dr. Akhavi Laboratory Co, Tehran, Iran

The role of green tea (Camellia sinensis) in the management of AndroGenetic Alopecia (AGA): A review

Alopecia is a condition that impacts over 50% of the global population. The Food and Drug Administration (FDA) only approved topical minoxidil and oral finasteride for prevention of hair loss, and hair regrowth. Numerous in vitro and in vivo studies on active herbal ingredients suggest the herbal active ingredients may help control hair loss when used alone, together, and in combination with synthetic anti-hair loss medicines. For over 100 years, thyme, lavender, rosemary, and cedar wood essential oils have traditionally used to treat hair loss. According to current researches about topical green tea in the prevention and hair re-growth, this plant may be a suitable and relatively reliable alternative to chemical drugs such as minoxidil and finasteride, Green tea contains polyphenol compounds called catechins. Catechins have a significant anti-hair loss due to their effect on the Dermal Papillae Cells (DPCs); DPCs are specialized fibroblasts that control the hair growth cycles. This article reviews the potential impact of green tea (Camellia sinensis) in reducing hair loss, hair re-growth, and its particular effect on dermal papillae.

Biography

Farshad Akbarnejad completed his DVM from Shahid Chamran University of Ahvaz. He is the head of the scientific and educational department of Dr. Akhoi Laboratory Company of Iran. He has more than 30 publications and 10 books. His professional activities are in the field of medicinal plants and cosmetic formulations, in which he has been active for more than 16 years.



Farshad Akbarnejad
Scientific Department, Dr. Akhavi Laboratory Co, Tehran, Iran

Malva Sylvestris L. Application in dermatology

Malva Sylvestris (MS) L. has been used as an herbal drug in Iran, which is referred to as Panirak. MS blossoms are used to treat eczema, cuts, wound infections, and skin inflammation problems. MS leaves and flowers are soothing and useful for sensitive skin areas. It is used as a topical poultice to reduce swelling and eliminate toxins. This article reviews its properties for skin problems. Scientific search engines such as PubMed, Wiley, Springer, ScienceDirect, and Google Scholar were used to collect data on Malva sylvestris. The purpose of this review is to highlight the dermatological uses of Malva sylvestris.

Keywords: Malva Sylvestris, Herbal Drugs, Anti-Bacterial, Anti-Inflammatory, Eczema, Anti-Oxidant.

Biography

Farshad Akbarnejad completed his DVM from Shahid Chamran University of Ahvaz. He is the head of the scientific and educational department of Dr. Akhoi Laboratory Company of Iran. He has more than 30 publications and 10 books. His professional activities are in the field of medicinal plants and cosmetic formulations, in which he has been active for more than 16 years.



Iliana Ivanova[1]*, Yoanna Kostova[2], Lilia Yordanova[1], Albena Bachvarova Nedelcheva[2]

[1]Faculty of Biology, Sofia University St. Kl. Ohridski, 8 Dragan Tsankov Str., 1164 Sofia, Bulgaria

[2]Institute of Metal Science, Equipment and Technologies with Hydro- and Aerodynamics Centre Acad. A. Balevski, Bulgarian Academy of Sciences, Shipchenski Prohod Str., 67, 1574 Sofia, Bulgaria

Sol-gel synthesis of silica-poly (vinylpyrrolidone) hybrids with improved antibacterial properties

It is well known that inorganic nanoparticles are highly stable and multifunctional, their biodegradability and biocompatibility have been disputed. Additionally, organic carriers are known for their high biocompatibility and biodegradability, but low stability and single functionality. The advancements in material science catalysed the fabrication of organic-inorganic hybrid nanoparticles which combine desirable properties of organic and inorganic materials to overcome the above mentioned disadvantages. On the other hand, the increasing resistance of human-threatening bacterial strains to traditional antibacterial treatments encourages the consideration of new infection control strategies. The combination of antibiotics and composite nanoparticles multiplies the efficacy of antibiotics against resistant bacteria. In addition, nanoparticle-antibiotic conjugates reduce the amount of both agents in the dosage, which reduces toxicity and increases antimicrobial properties.

The present work deals with sol-gel synthesis of silica - poly (vinylpyrrolidone) hybrid materials. The nanohybrids (Si-PVP) have been prepared using an acidic catalyst at ambient temperature. Tetramethyl Ortosilane (TMOS) was used as a silica precursor. Poly (Vinylpyrrolidone) (PVP) was introduced into the reaction mixture as a solution in ethanol varying its concentration between 5 and 20 %. The XRD established that the as – prepared materials are amorphous. The gel derived nanopowders were characterized also by SEM, TEM and AFM techniques. The efficacy of Si/PVP nanoparticles as a potential antimicrobial agent against a wide range of bacteria, including those with novel resistance mechanisms using agar diffusion and spot test has been evaluated. Furthermore, we are monitoring the direct bactericidal effects and synergetic effect of the nanoparticles in combination with different antibiotics in liquid media, with the aim of reducing the Minimum Inhibitory Concentration (MIC) and Minimum Bactericidal Concentration (MBC). Combined therapy can significantly reduce the concentrations of both the antibiotic and the nanocomposites, but also eliminate the antibiotic resistance of the pathogen. These findings suggest that the newly synthesized Si/PVP nanoparticles may be a new, effective and broad-spectrum antibacterial agents, even at lower doses than those currently used in clinical trials to treat bacterial infections.

Biography

Dr. Iliana Ivanova finished Medical college in Plovdiv in 1979. She finished her Biochemistry and Microbiology Master's degree at Sofia University Saint Kliment Ohridski in 1986 (diploma thesis on Aspergillus niger acid production) and her Ph.D. degree in Microbiology Microflora of oil-field Tyulenovo and its application in 1994. In 2009 Dr. Ivanova started to test the antimicrobial activity of ZnO thin films and now has more than 50 articles published in international journals and books. Her interests are in the antimicrobial activity of nanoparticles and nanocomposites and their medical application.



Jerry T. Thornthwaite
Cancer Research Institute of West Tennessee Daniel Strasser, Olufemi Akanni

Nutrananospheres for nutraceutical delivery systems

About 90% of all compounds in the pharmaceutical drug market have solubility in water. About 60% of people over 60 and 40% of all ages have struggled to take solid medicines, such as tablets or capsules. We have developed new pharmacology with our NutraNanoSpheres™ (NNS) approach by miscellizing nutraceuticals, pharmaceuticals, and peptides to form stable NNS products. The NNS are completely soluble in water and are heat stable. We use a natural fatty acid without organic solvents to encapsulate nutraceuticals in sub-microscopic micelles in which over 500 can stretch across a human red cell as for curcumin. The NNS are not degraded in the stomach, pass into the bloodstream, and can cross the blood-brain barrier to offer high bioavailability. We have used a variety of NNS formulations to cure Malaria using an in vivo vaccination process in babies, treat antiviral assaults, provide formulations for cancer, heart disease, brain dysfunction, and energy enhancement. The NNS offer time-released mixtures of compounds that operate synergistically with the assurance that the NNS are stable and do not interact with each other. Examples of our applications of this technology include multilayered NNS for time-released Vitamin C, water-soluble antimalaria treatment for babies provided a milk bottle with a 93% cure rate, rapid recovery from severe COVID-19, a brain energy formulation, and treatment of Choline deficiency in pregnant women.

Biography

Jerry T. Thornthwaite completed his chemistry doctoral program in 1975 at Florida State University with a research emphasis in biophysics. He has performed extensive research in instrumentation, reagents, and clinical applications in flow cytometry, image analysis, and luminometry. He helped to conduct grants from NASA, ACS, DARPA, NIH, and McCormick Research, among others. In 1972, he discovered what is now recognized as the Natural Killer Cell (NKC) and has published significant research in prophylactically and therapeutically enhancing NKC activity. In addition, he developed a malaria treatment in Haiti and Nigeria, which cured over 90% of the patients without recurrence. He started the two largest Immuno-Oncology Laboratories at Cedars Medical Center and Baptist Hospital in Miami and was the Clinical Laboratory Director. He has published over 70 papers and holds ten patents.



Jinsong Wu
University of Chile, 8370451, Chile

Environmental sustainability and intelligence as well as general green technologies

Although the term of green has been often used to refer to energy consumption reduction or energy efficiency by many people and literatures, green actually should refer to environmental sustainability in more general senses. Environmental sustainability issues have been important topics for recent years, which has impacted and will further impact individuals, enterprises, governments, and societies. Environmental sustainability is not simply regarding reducing the amount of waste or using less energy, but relevant to developing processes leading to completely sustainable human society in the future. The long term consequences of the relevant serious issues have not yet been fully forecasted, but it has been generally accepted in many communities that immediate responses are necessary. From 30 November to 12 December 2015, the 21th United Nations Climate Change Conferences of the Parties (COP 21) was held in Paris, France, as the a historical breakthrough and milestone towards securing the future Earth, a global agreement on the reduction of climate change, the text of which represented a consensus of the representatives of more than 193 countries attending it, which was a profound milestone for global environmental sustainability. Nowadays there is another significant tendency on data driven intelligence. This talk would discuss the history, technical issues, challenges, and new trends of data driven environmental sustainability and Intelligence. Further this talk will extend the view to general green technologies.

Audience Take Away Notes

- Environmental sustainability is not simply regarding reducing the amount of waste or using less energy, but relevant to developing processes leading to completely sustainable human society in the future
- The long term consequences of the relevant serious issues have not yet been fully forecasted
- Nowadays there is another significant tendency on data driven intelligence
- This talk would discuss the history, technical issues, challenges, and new trends of data driven environmental sustainability and Intelligence
- Further this talk will extend the view to general green technologies

Biography

Jinsong Wu received the Ph.D. degree from the Department of Electrical and Computer Engineering, Queen's University, Kingston, Ontario, Canada, in 2006. He is proposer (2021) the Founder (2022) and Founding Editor-in-Chief (2022-present) for the new international journal, Green Technologies and Sustainability (GTS), KeAi. He received 2020 IEEE Green Communications and Computing Technical Committee (TCGCC) Distinguished Technical Achievement Recognition Award, for his outstanding technical leadership and achievement in green wireless communications and networking. He was the leading editor and a coauthor of the comprehensive book, entitled Green Communications: Theoretical Fundamentals, Algorithms, and Applications (CRC Press, September 2012). He received the 2017, 2019, and 2021 IEEE System Journal Best Paper Awards.



Robin Ramos[1], Anthi Karaiskou[1], Candice Botuha[2], Sadek Amhaz[1], Michele Salmain[2], Joelle Sobczak Thepot[1]*

[1]Centre de Recherche Saint Antoine, Sorbonne Universite, INSERM, Paris, France
[2]Institut Parisien de Chimie Moleculaire, Sorbonne Universite, CNRS, Paris, France

Half-sandwich iridium(III) complexes mechanism of action for anti-cancer therapy: Cytoskeletal proteins and heat-shock proteins as privileged protein targets

The identification of intracellular targets of anticancer drug candidates provides key information on their mechanism of action. (C^N)-chelated half-sandwich iridium(III) complexes are currently being investigated for their anti-proliferative and pro-apoptotic capacity, both linked to their pro-oxidant activity and ability to raise intracellular levels of hydrogen peroxide, to which tumour cells are more sensitive. We have previously shown that this class of molecules is also capable of reacting with amino acids and forming protein adducts in the cellular environment, thus providing a new mechanism of action explaining their cytotoxicity. I will discuss the different approaches we have undertaken to analyse the intracellular fate of such complexes, either in an unbiased manner, through X-ray fluorescence imaging of iridium, or through chemical modification allowing indirect fluorescent imaging (molecule appended by Bodipy and use of click-chemistry). I will also discuss (i) our recent identification of a range of protein targets, through a click-and-capture assay with a clickable half-sandwich (C^N) iridium(III) complex, and (ii) how the iridium-based complex modifies chaperone proteins involved in protein folding and the actin cytoskeleton. Collectively, these results open a new avenue for the development of half-sandwich iridium-based anticancer drugs.

Audience Take Away Notes

- The presentation will present robust methods to visualize a metal-based drug in cellulo (XRF) but also methods that can be expanded to metal-devoid drugs, in order to visualize the molecule in cells (through click chemistry) and to colocalise its targets (with a proximity-ligation assay)
- These approaches are particularly suited to chemists interested in medicinal chemistry and preclinical approaches
- This research provides valuable insights that other faculty could use to expand their research or teaching
- This provides a practical solution to a problem that could simplify or make a designer's job more efficient
- For example, through the illustration of a proteomic approach to click-and-capture protein targets of a given drug
- The approaches and results are relevant to studies dealing with chemical reactivities of molecules in vivo in the cellular context (through oxidative and electrophilic stresses)

Biography

Dr. Sobczak studied Biochemistry at ENS Paris, France and received her MD in 1983. She then joined the research group of the late Professor Duguet at P&M Curie University, Paris and received her PhD in Molecular Biology in 1988. After brief stays as a postdoctoral fellow, notably at the Institut Necker Enfants-Malades (supervisor Prof. Brechot), she was appointed to the Department of Biochemistry at P&M Curie University, Paris in 1991 as an Assistant Professor. She was promoted to full Professor of Cell Biology at Sorbonne University, Paris in 2000. She has published more than 40 research articles in SCI(E) journals.



Karen J. Cloete[1,2]*, Nandipha L. Botha[1,2], Ziga Smit[3,4], Kristina Isakovic[4], Gabriel Kaningini[1,2], Thobo Motlhalamme[1,2], Mahmood Akbari[1,2], Razieh Morad[1,2], Itani Madiba[1,2], Admire Dube[5], Oladipupo Moyinoluwa David[5], Primoz Pelicon[4], Malik Maaza[1,2]

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Multidimensional analysis of nanofertilizers

Nanofertilizers are poised to revolutionize modern agriculture by offering a range of benefits over traditional fertilizers. Their nanoscale particles provide a significantly higher surface area, leading to improved nutrient solubility and availability in the soil. This enhanced availability ensures that plants can efficiently absorb and utilize nutrients, reducing wastage and enhancing nutrient use efficiency. Nanofertilizers can also be engineered with controlled-release mechanisms, ensuring a gradual and sustained nutrient supply to plants throughout their growth stages. This targeted delivery not only optimizes plant nutrition but also minimizes nutrient leaching, runoff, and volatilization, thereby reducing environmental pollution. Moreover, nanofertilizers can be customized to specific crop and soil requirements, promoting soil health and supporting sustainable agricultural practices. Overall, nanofertilizers hold immense promise in improving crop yields, reducing fertilizer usage, and mitigating environmental impacts in modern agriculture. This presentation will delve into the multidimensional analysis of nanofertilizers, encompassing various scientific perspectives and analytical techniques to assess their efficacy and effect on plants. More specifically, results from studies focused on phytosynthesized nanofertilizers supported by computational modelling on the physiology of bean seeds will be discussed. The work encompassed nanofertilizer development, application to seeds, and analysis using multidimensional accelerator and benchtop techniques for investigating the nanofertilizer's effect on the bean seed's ionome and amino acid metabolism. The data shows that the nanofertilizer exhibited a unique distribution pattern in seeds that may also boost its potential as a seed protective, nutritive, and growth promoting agent in light of its effect on seed physiology. Through this exploration, the presentation aims to underscore the potential significant role of nanofertilizers in advancing sustainable and high-yielding agricultural practices for future food security and environmental stewardship.

Audience Take Away Notes

- Novel agro-technologies in the form of agro-nanotechnology
- The development and application of nanofertilizers to plants and their effect on plant physiology
- The importance of multidisciplinary research to address key challenges in agriculture

Biography

Karen is currently a senior researcher at the UNESCO-UNISA Africa Chair in Nanosciences and Nanotechnology Laboratories - University of South Africa and the Nanosciences African Network - iThemba Laboratory for Accelerator Based Science - National Research Foundation as well as a member of Nanoenergy for Sustainable Development in Africa.



Kazeem Sholotan Oluwatoyin Sholotan*, Bello H. O, Ajayi J. B, Nosiru D. S, Lawal D, Adedeji S. M

Ogun State Institute of Technology Igbesa Department of Science Laboratory Technology, Nigeria

Comparative analysis of synthesized waltheria indica leaf and Euphorbia maculata herb zinc nanoparticle

Zinc nanoparticles of Euphorbia maculata and Waltheria indica were synthesized and analyzed for their optical properties using UV/V is spectrophotometer (peak absorbance at 380nm) and Fourier Transmission Infra-red Spectrophotometer (3200 and 3295cm^{-1} signifies OH; 2098cm^{-1} represent CH_2, 1636cm^{-1} represent C=O while the stretch around 600cm^{-1} could be attributed to the vibrations of elongation and of deformation of vibratory ZnO). The surface morphology of the synthesized Zinc Nanoparticles (Zn-NPs) were also taken into consideration using Q250 Scanning Electron Microscope from FEI Eindhoven the Netherland (E. maculata Zn-NP has an average diameter size of 3.766 nm while W. indica Zn NP has an average diameter size of 11.87 nm). Furthermore; the antimicrobial activity of the synthesized nanoparticles were compared with the diluted crude extracts of E. maculata and W. indicaas well as zinc sulphate hepta-hydrate solution while commercially available antibiotics were used as control against five bacteria isolates namely Staphylococcus aureus, Escherichia coli, Proteus mirabilis, Klebsellia pneumoniae and Pseudomonas aeruginosa as well as two fungi isolates namely Aspergillus flavus and Aspergillus niger; thus exhibiting varying susceptibility range against each isolates. Anticoagulant activities of the nanoparticles were compared with that of zinc sulphate solution and the respective crude extracts while EDTA was used as control with anticoagulation value ranging from 2 minutes to 240 minutes. Antioxidant activities of the nanoparticles, zinc sulphate solution and the respective crude plant extracts were compared with that of ascorbic acid.

Keywords: Nanoparticle, EDTA, Spectrophotometer, FTIR, Synthesis.

Biography

Sholotan Kazeem is currently an undergraduate Educator at Ogun State Institute of Technology Igbesa, where he teaches Microbiology and other related subjects with major interest in Research and Innovation. He had completed his Primary Education from 1991 – 1997 at St. Mary Nursery & Primary School and his Secondary Education from 1997 - 2003 at Awori College Ojo, Lagos. He worked as a Mobile (GSM) Technician from 2003 - 2006 at Phem-Tech Consulting. He also completed National Diploma (SLT) from 2006 to 2008 at Gateway Polytechnic Igbesa, currently known as Ogun State Institute of Technology Igbesa. He also worked as ICT Essential from 2007-2008 in Gateway Polytechnic Igbesa) and as Industrial Trainee from 2008 - 2010 at Nestle Nig Plc. He Completed his Higher National Diploma in Microbiology from 2009 - 2011 at Moshood Abiola Polytechnic Abeokuta, BSc. (Microbiology) in 2024 at Federal University of Oye Ekiti, Postgraduate Diploma in Microbiology from 2014 – 2016 at Covenant University Ota and MSc in Microbiology from 2016 - 2018 at Fountain University Osogbo.



Kung Chung Yuan
National Chung Hsing University, Taiwan

The formation of the four-way symmetric translational tiles (crystal) and corresponding unit cells

Four-way symmetric translational tiles are typically observed in crystals with a fourfold rotational symmetry. These tiles can form various types of crystal lattices, depending on the arrangement of the tiles and the choice of unit cell. A Penrose collage may possess (so defined) five-fold rotational symmetry (on a specific point) and reflection symmetry, but not translational symmetry. Given the widespread acceptance of (so defined) five-fold rotational symmetry as a distinguishing feature of Penrose tiles, it appears no one believe that four-way symmetric Penrose tiles can be easily made. The most intriguing discovery is that Penrose tile has an infinite capacity for self-extension in translation, and with all six different inner-structure decagons coexisted.

The unlimited unit cell can be easily extracted from the tiling (crystal) that by coupling scheme of different Pentangular Penrose tiles, that may be very useful to image the structures of new quasi crystals.

Audience Take Away Notes

- The definition of crystal
- Build an Imagination of quasicrystal
- Solid state physics
- It helps to draw an infinite large Penrose tiles, and perceives what it looks like at infinity
- You may make an unlimited combination with basic circular and Pentagonal shape Kung's clusters
- It will make a lot of money, if printed in 3mX3m, with million diamonds, and all six different Decagons coexisted. At least one million with my signature

Biography

Dr. Kung graduated from National Tsing Hua University 1969 and 1972 with BS and MS degree in physics, university of Alabama in Huntsville 1974 in physics and Northwestern university 1979 in material science. Post doctor at Georgia Tech and research science at Lawrence laboratory. With about 6 years experiences in US industries Fairchild and National Semiconductor and work for ITRI (Taiwan) since 1987 and worked for National Chung-Hsing University electric engineering department since 1991 to 2016 (retired).



Malachi Warneke
University of California, Los Angeles

The formation of the periodic translational penrose tiles (crystal) and their corresponding unit cells

Utilizing a variety of permutations and combinations of coupling skills, binary circular Penrose tiles of translation mirror symmetry have been constructed and their corresponding unit cells have also been defined. A tessellation of unit cells can perceive translational mirror Penrose tiles of infinite size and the number of such unit cells is infinite. A penrose tube is made by rolling- up tiles in four directions, and a smallest Penrose football shape can be made using unit cell.

Key words: Decagon, Penrose Tiling, Binary Tiling System, Circular Shape, Translational Periodic Penrose Tiles, Unit Cell.

Biography

Malachi Warneke is a second year chemistry major at the University of California, Los Angeles. He conducts research under Richard Kaner working on Zinc ion batteries. In his free time, he enjoys serving at his church, playing soccer, and practicing viola.



Maria Cristina Gamberini[1]*, Al Otaibi, Jamelah .S[2], Mary Y. Sheena[3], Mary Y. Shyma[3], Kratky, Martin[4], Vinsova Jarmila[4]

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[4]Department of Organic and Bioorganic Chemistry, Faculty of Pharmacy in Hradec Kralove, Charles University, Akademika Heyrovskeho 1203, Hradec Kralove, 500 05, Czech Republic

Study of several antimicrobials, physical proprieties

Theoretical and experimental study were conducted on several antimicrobials (ex: p-tolyl 2-Acetamido-3-(4-Fluorophenyl)Propanoate (AFP), novel bioactive molecule 2-(3-Bromobenzoyl)-n-Methylhydrazine-1-Carboxamide (BMC), (E)-4-methoxy-N′-(2-(Trifluoromethyl)benzylidene) benzohydrazide (EMT) etc etc). Density Functional Theory (DFT), Time Dependent (TD)-DFT and Surface Enhanced Raman Scattering (SERS) studies are reported for the adsorption on silver hydrosols. SERS at various concentrations are discussed and their orientation changes with concentration are studied. After adsorption on silver surface, the structural properties of antimicrobials exhibit somtetimes modifications, indicating an interaction between them and Ag6 cluster. On some samples molecular docking are performed to find their ability to bind to target proteins. Silver nanoparticles are successfully used for the treatment of different diseases alone or in association with other active components and the incorporation of antimicrobials with silver nanocolloids could act as a nanodrug delivery system. The findings presented could futhermore help in the construction of more dependable SERS sensors by thoroughly describing the concentration-dependent profile of analyte orientation.

Keywords: Antimicrobials, SERS Raman, DFT, Docking.

Audience Take Away Notes

- Identification and characterizations of antimicrobials
- Application of Raman spectroscopy in antimicrobials analysis
- Notions on SERS colloids

Biography

Maria Cristina Gamberini has a degree in Chemistry, her first period abroad at the Polytechnic of Lausanne has been dedicated to the study of nanomaterials using spectroscopic techniques, studies of pigments and minerals. She is professor at the University of Modena and Reggio Emilia in the Chemistry Laboratory. Her main scientific interest is linked to the experimentation of the Raman Spectroscopy Technique on simple or complex matrices. For years she has studied crystals and cocrystals and polymorphs. The study and characterization of inorganic samples in collaboration with various international groups has allowed the publication of numerous articles in international journals. She has been a speaker at several international conferences. The study is currently focused on Raman spectral identification and characterization of inorganic and also organic samples.



Maffezzoni .M. B. R[1], Prato .V. J[1], Ferrari .V[1,2], Marisaldi .L[3], Ferrari .A[3], Prevedelli .D[2], Bergami .E[1,4], Maria Cristina Gamberini[1]*

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Microplastics in marine environments: Raman identification and characterization

Over the past decade, numerous studies have extensively examined the issue of plastic waste accumulation in marine environments. Of growing concern is the widespread dissemination of microscopic plastic particles, posing a significant threat to marine life. Plastic debris undergoes mechanical and biological degradation, leading to the formation of microplastics, defined as particles smaller than 5 mm. The identification and quantification of microplastics present a formidable challenge due to their minute size and complex composition. Raman microscopy emerges as an indispensable tool for analyzing extremely small microplastics (<20 um). As per the World Health Organization's guidelines, plastic particles smaller than 150 μm have the potential to enter the human body, raising health concerns. Given their diminutive dimensions, microplastics may be ingested by marine fauna, with uncertain ramifications for their health. In this study, Microplastics (MPs) extracted from jellyfish and Ctenophora were analysed using Raman spectroscopy. The spectra were successfully distinguished through a combination of available databases and a spectral reference database of MPs established in-house. In this study, the primary MPs identified were Polyethylene (PE) and Polyethylene Terephthalate (PET). PE, being one of the most used plastics, emerged as the predominant type. PET, another prevalent plastic, was also notably present among the microplastic samples analysed. Many of the Microplastics (MPs) exhibit significant degradation and alteration, posing challenges for their analysis and identification. Therefore, there is a pressing need for more in-depth studies and comprehensive databases to effectively address these complexities. Furthermore, considering the challenges posed by the degradation and modification of microplastics, uniformity and harmonization of experimental conditions become even more imperative. Consistent methodologies not only aid in overcoming analytical complexities but also contribute to the reliability and compatibility of data collected. By ensuring standardization across studies, researchers can build comprehensive databases that serve as invaluable resources for tackling the issue of microplastic pollution effectively.

Audience Take Away Notes

- Identification and characterizations of microplastics
- Application of Raman spectroscopy in microplastics analysis
- Practical applications on real samples

Biography

Maria Cristina Gamberini has a degree in Chemistry, her first period abroad at the Polytechnic of Lausanne has been dedicated to the study of nanomaterials using spectroscopic techniques, studies of pigments and minerals. She is professor at the University of Modena and Reggio Emilia in the Chemistry Laboratory. Her main scientific interest is linked to the experimentation of the Raman Spectroscopy Technique on simple or complex matrices. For years she has studied crystals and cocrystals and polymorphs. The study and characterization of inorganic samples in collaboration with various international groups has allowed the publication of numerous articles in international journals. She has been a speaker at several international conferences. The study is currently focused on Raman spectral identification and characterization of inorganic and also organic samples.



Tomy Hos, Miron V. Landau, Moti Herskowitz*

Chemical Engineering Department, Blechner Center for Industrial Catalysis and Process Development, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel

Hydrogenation of CO_2 on Fe-based catalysts: Preferred route to renewable liquid fuels

Catalytic hydrogenation of CO_2 can be conducted either in one-pot (CO_2 hydrogenation) or in two-stages (RWGS and CO hydrogenation). Its configuration consists of either three reactors in series with interim water removal (one-pot process) or CO_2 separation and recycling (two-stage process) to reach high CO_2 conversion. The two-stage process enables to reach optimal H_2/CO and temperature in the hydrogenation reactor to yield higher productivity while minimizing production of aqueous phase, which offset the advantages of the one-pot process. The techno-economic study determined that there is no apparent advantage in operating the hydrogenation reaction in one stage at current green hydrogen prices. The decision between the two routes should be based on catalyst stability and selectivity towards desired products. Blending 10% of liquid product from both processes with fossil fuels at current prices increases the fuel production cost by 30% that can be offset by higher carbon pricing or equivalent incentives.

Biography

Moti Herskowitz is professor of chemical engineering and researcher in the fields of advanced materials, heterogeneous catalysis, and reaction engineering and renewable fuels. He served, among other positions, as Vice-President for R&D at the Ben-Gurion University from 2003 to 2014. Moti established the Blechner Center for Industrial Catalysis and Process Development in 1995 and has led scientific programs and technology development work ever since. Moti has published over 160 papers and 27 patents based on basic and applied research, related to advanced catalytic materials, processes and their application in the production of novel renewable fuels and chemicals.



Ola Michałkiewicz[1]*, Iwona Nowak[1], Iwona Rykowska[1], Rafał Nowak[2]

[1]Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznanskiego 8, 61-614 Poznan, Poland

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The potential of drug release systems in the treatment of ocular diseases

Ophthalmic drug delivery is an essential important area of research that aims to improve the efficacy and convenience of treatment for various eye conditions. Therapies based on applying of eye drops are the most commonly used form of treatment, constituting approximately 90% of the preparations available on the market. However, due to the unsatisfactory results of their use, including low bioavailability of approximately 5%, several efforts were made to develop systems that release drugs in a controlled manner and are characterized by higher bioavailability of active substances.

The use of carriers such as Contact Lenses (CLs) in ophthalmological therapies allows for a significant extension of the residence time of drug molecules on the cornea. In the case of eye drops it is a few minutes, while in the case of CLs, it is several hours. Active substances can be applied to their surfaces using various techniques. The dip coating process is the most commonly used method.

Drug Modified Contact Lenses (DMCL) are a promising therapeutic tool, especially for patients struggling with chronic eye diseases. Their matrices are modified with various active substances, including Cyclosporine A (CyA). CyA was first isolated in Norway in 1970 from a fungus called Tolypocladium Inflatum. It is an immunosuppressive drug with a broad spectrum of action, which is why it is used in many fields of medicine, among others in ophthalmology, in the symptomatic treatment of Dry Eye Syndrome (DED).



Figure 1 Cyclosporine A

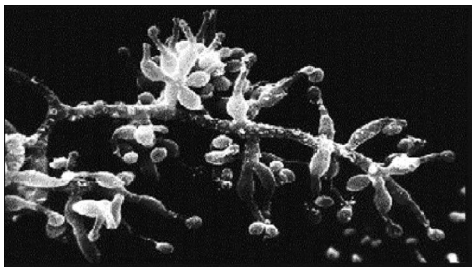


Figure 2 Tolypocladium Inflatum [1]

In our presentation, loading techniques of Cyclosporine A on drugstore contact lenses will be proposed. Obtained drug release profiles for different drug loading parameters will also be discussed.

Audience Take Away Notes

- Presentation of the benefits of using controlled Drug Delivery Systems (DDS)
- Discussion of selected research results obtained during the modification of selected polymer carriers with cyclosporine A
- A potential to expand research on DDS modified with various active substances and techniques by other research groups

Biography

Mrs. Ola studied Chemistry at the Adam Mickiewicz University, Poland and graduated with an MSc in 2022. Then she joined the research group of Prof. Iwona Rykowska at the same institution. Currently, she is involved in research on the development of controlled release systems of selected ophthalmic drugs (DDS) in the form of Drug Modified Contact Lenses.



Osman Adiguzel
Department of Physics, Firat University, Elazig, Turkey

Thermomechanical processes and transformations in shape memory alloys

Shape memory alloys take place in a class of advanced structural materials by exhibiting dual memory characteristics, shape memory effect and superelasticity with the recoverability of two shapes at different conditions, in the β-phase region with chemical composition. Shape memory effect is initiated with thermomechanical processes on cooling and deformation and performed thermally on heating and cooling, with which shape of the material cycles between original and deformed shapes in reversible way, and this behavior can be called thermoelasticity. This phenomenon is governed by the thermomechanical transformations, thermal and stress induced martensitic transformations. Thermal induced martensitic transformation occurs on cooling with cooperative movement of atoms in <110 > -type directions on {110} - type plane of austenite matrix, along with lattice twinning and ordered parent phase structures turn into the twinned martensite structures, and twinned structures turn into detwinned martensite structures by means of stress induced martensitic transformations with deformation. Superelasticity is performed in only mechanical manner with stressing and releasing the material in elasticity limit at a constant temperature in the parent austenite phase region, and shape recovery occurs immediately upon releasing, by exhibiting elastic material behavior. Superelasticity is also result of stress induced martensitic transformation, and the ordered parent phase structures turn into the detwinned martensite structures with stressing. It is important that lattice twinning and detwinning reactions play important role in martensitic transformations.

Copper based alloys exhibit this property in metastable β-phase region, which has bcc-based structures. Lattice twinning is not uniform in these alloys, and the ordered parent phase structures undergo the non-conventional layered structures with martensitic transformation. These layered structures can be described by different unit cells as 3R, 9R or 18R depending on the stacking sequences on the close-packed planes of the ordered lattice.

In the present contribution, x-ray diffraction and electron diffraction studies were carried out on copper based CuZnAl and CuAlMn alloys. X-ray diffraction profiles and electron diffraction patterns exhibit super lattice reflections. Critical transformation temperatures of these alloys are over the room temperature. The specimens were aged at room temperature, and a series of x-ray diffractograms were taken during aging. X-ray diffractograms taken in a long-time interval show that locations and intensities of diffraction peaks change with the aging time, and this result refers to the redistribution of atoms in diffusive manner.

Keywords: Shape Memory Effect, Martensitic Transformation, Thermoelasticity, Superelasticity, Twinning, Detwinning.

Audience Take Away Notes

- Shape memory alloys are multifunctional materials and used in many fields from biomedical to the building industry. In principle, I introduce the basic terms and definitions related to shape memory effect, and introduce the experimental studies performed on the alloy specimens

Biography

Dr. Adiguzel graduated from Department of Physics, Ankara University, Turkey in 1974 and received PhD-degree from Dicle University, Diyarbakir-Turkey. He has studied at Surrey University, Guildford, UK, as a post-doctoral research scientist in 1986-1987, and studies were focused on shape memory effect in shape memory alloys. His academic life started following graduation by attending an assistant to Dicle University in January 1975. He became professor in 1996 at Firat University in Turkey, and retired on November 28, 2019, due to the age limit of 67, following academic life of 45 years. He supervised 5 Ph.D-theses and 3 M.Sc-theses and published over 80 papers in international and national journals; He joined over 120 conferences and symposia in international level with contribution. He served the program chair or conference chair/co-chair in some of these activities. Also, he joined in last six years (2014-2019) over 60 conferences as Keynote Speaker and Conference Co-Chair organized by different companies. Additionally, he joined over 120 online conferences in the same way in pandemic period of 2020-2022. Dr. Adiguzel served his directorate of Graduate School of Natural and Applied Sciences, Firat University, in 1999-2004. He received a certificate awarded to him and his experimental group in recognition of significant contribution of 2 patterns to the Powder Diffraction File–Release 2000. The ICDD (International Centre for Diffraction Data) also appreciates cooperation of his group and interest in Powder Diffraction File.



Radoslaw Banasz*, Monika Walesa Chorab

Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznanskiego 8, 61-614 Poznan, Poland

Investigation of phenyl and triphenylamine-based star-shaped viologens for electrochromic applications

The branched viologens (so-call star-shaped) are organic compounds derived from 1,1'-di(hydrocarbyl)-4,4'-bipyridinium salt, which contain three or more pyridine rings connected to a central core. The implementation of the branched unit instead of linear one results in obtaining star-shaped compound. These viologens have attracted a greater interest in recent years due to their clearly different properties compared to the linear viologens. Switching between different redox states results in a very distinct color changes and this is the reason why they are intensively studied in terms of their electrochromic applications. It is expected that the branched compounds containing three N-substituted pyridine rings will undergo more oxidation/reduction processes and thus exhibit more colors during electrochemical oxidation/reduction.

In our research the two star-shaped viologens containing 1,3,5-substituted phenyl group and triphenylamine moieties with n-hexyl chains were synthesized and characterized using spectroscopic methods (^{1}H NMR, ^{13}C NMR, HR-ESI-MS). The compounds are N-substituted with n-hexyl chains what increases their solubility in organic solvents. This allowed for investigation solvatochromic properties of the triphenylamine-based viologen. The electrochemical and spectroelectrochemical measurements of the branched compounds were also investigated. Both star-shaped viologens indicate promising optical properties and these molecules could be used as the active materials in electrochromic applications.

Acknowledgments: This scientific work has been supported from the budget for science in the years 2020–2024, by Ministry of Science and Higher Education, Republic of Poland, as a research project under the Diamond Grant program no. DI2019/0164/49.

Audience Take Away Notes

- Participants will gain knowledge about viologens and their unique possibilities of applications in modern technology
- The presentation will provided information about electrochemical and spectrochemical measurements to characterize viologens in that other scientists could use the methods to expand their research
- The audience will get to know the two novel star-shaped viologens containing 1,3,5-substituted phenyl group and triphenylamine moieties with n-hexyl chains as a active materials electrochromic applications

Biography

Mr. Radoslaw Banasz studied Chemistry at the Adam Mickiewicz University in Poznan, Poland and graduated as MSc in 2021. He joined the research group of Prof. Monika Walesa-Chorab in 2017 at the same Institution. Mr. Banasz is a PhD student in the discipline of Chemical Science. He conducts research which is supported by Ministry of Science and Higher Education, Republic of Poland under the Diamond Grant program no. DI2019/0164/49. His currently research focus on synthesis and characterization of viologens as functional materials for applications in electrochromic devices. He is an author and co-author of 6 research articles in SCI(E) journals.



Rajiv Kashyap[1,2]*, Ramesh K Sharma[2], Martin J. Taylor[3]

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Investigating the electrochemical potential for mesoporous sugarcane bagasse biochars as supercapacitors

The transformation of waste obtained from biomass into usable commodities with enhanced performance is an essential undertaking. In this work, we produced mesoporous biochars with customisable surface areas and pore structures from lignocellulosic biomass waste. Biochars were created by varying the feedstock and sacrificial templating agent (KOH) mass ratios, the resulting materials were characterized by FTIR, XRD, TGA, Nitrogen physisorption, Elemental Analysis and FESEM. Electrochemical measurements were then carried out to investigate the charge storage ability of the material through Galvanometric Charge-Discharge (GCD) and Cyclic Voltammetry (CV). It was found that the biochar's structure would develop upto a KOH concentration of 0.5 M before structural collapse took place, destroying the pore structure and diminishing the available surface area. Capacitance calculations show that a maximum charge storage ability was achieved (490 F g^{-1}) at a current density of 0.5 A g^{-1}, with the highest surface area biochar (1669 m^2 g^{-1}) and smallest pore size (2 nm). This biochar was found to exhibit a 93.2% retention rate after 2000 cycles, thus making it an excellent cycle stability material for supercapacitors. This translates to an energy density of 136.17 Wh kg^{-1} at a power density of 500 W kg^{-1}, when used in a redox electrolyte (KOH). Overall, capacitance was found to follow a downward trend with respect to structural collapse. This work offers a novel and sustainably strategy of producing customisable supercapacitor materials from biomass waste, as a result enable a wider application of these materials in the quickly developing and essential energy storage market.

Audience Take Away Notes

- To provide a new approach to sustainable energy storage options, the presentation shows how sugarcane bagasse waste may be converted into activated mesoporous carbon materials with improved electrochemical performance
- This study offers insightful information and useful approaches that other academics could apply to broaden their studies in fields about the use of biomass waste, the synthesis of carbon materials, characterization methods, and energy storage applications. This would enhance their research as well as their efforts to teach
- By showing how biomass waste may be converted into high-performance carbon materials for supercapacitor applications, this research provides a workable alternative and may make it easier for designers to find effective and sustainable energy storage solutions

Biography

Mr. Rajiv Kashyap is a master's graduate of Kurukshetra University, India in physics. He then became eligible for national exams such as JEST, GATE, BARC, and CSIR-JRF. This made it possible for him to enroll in Panjab University, Chandigarh, where he is now a research scholar in the Department of Materials Science, as part of their PhD program. He has recently been awarded a Commonwealth Split-Site Fellowship to study at the University of Hull in the United Kingdom to advance his studies in energy storage and hydrogen production using Net Zero solutions.



Prof.dr. Ruzumboy Eshchanov
Chirchik State Pedagogical University of Tashkent region, Uzbekistan

Theory of transformation in atomic and nucleon orbitals

An electron and other waves are Electromagnetic Wave Packets (EMWP) or energy depending on the state. Atomic, proton, and neutron orbitals, during transformation, form interatomic and internucleon bonds. Electrons of one atomic orbital are transformed into spherical, hemispherical, and sector-spherical electrons in an electromagnetic wave packet according to the principle of minimum total energy, and the direction of the molecular orbital depends on the state of the valence electron and is part of the atomic orbital. Electronic formulas for elements in a state of rest and an excited state have been developed.

An electromagnetic wave packet has a charge and spin, which has a closed continuous, uniform, stable, stationary form of electromagnetic wave and is located in a stationary atomic orbital in a single state or in pairs in a cell with opposite spins, in which the orbitals are divided, but in one orbital, the cells cannot be arranged in layers, that is, to intersect or overlap. An EMWP does not have a different shape, for example, dumbbell-shaped or ellipsoidal.

The formation of atomic and molecular orbitals occurs through pairing with the transformation of electron orbitals by high-order electromagnetic wave packets. Therefore, we propose the theory of transformation of electromagnetic waves as a new theory, with explanations, as well as the formation of equivalent chemical bonds from equivalent electrons. A chemical bond always has a single character and is not divided into σ- and π-bonds. The spin of an electron, positron or gamma wave means the formation of a bond between identical electromagnetic wave packets, such as the formation of an atomic, proton or neutron bond.

Keywords: Electron, Positron, Gamma Waves, Neutron, Proton, Spin, Theory of Transformation.

Biography

Ruzumboy Eshchanov is a distinguished academic based in Uzbekistan, specializing in chemistry, sustainable development, education and research policy. He serves as a Professor of Chemistry at Chirchiq State Pedagogical Institute of Tashkent Region. Prof. Eshchanov obtained his education from Tashkent State University and defended his doctoral degree at the Moscow State Institute of Fine Chemical Technologies. Ruzumboy Eshchanov has a long record of managerial experience in education and science. He has served as the dean of the Natural Sciences faculty for 14 years and as a rector of the Urgench State University for eight years. Along with teaching at various levels starting from high school to postgraduate programs, Prof. Eshchanov has been active in various research fields, particularly focusing on physical chemistry, land and water use optimisation and education and research policy analysis of Uzbekistan. He has built long-lasting international academic and scientific collaborations with various prestigious institutions. Eshchanov's contributions extend to publications in reputable journals and participation in international collaborative research. He has authored and co-authored several significant scientific and policy papers and book chapters. Ruzumboy Eshchanov is currently working in the field of bonding of atomic and sub-atomic particles.



Sergey Suchkov[1-7]*, Noel Rose[8-10], Aleks Gabibov[11,12], Harry Schroeder[13]

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Antibody-proteases as natural and translational tools of the next step generation to be applied for biodesign-driven biotech and personalized and precision medical practice

Biomarkers may aid in diagnosing disease, predicting disease onset, and selecting appropriate therapy. Meanwhile, Antibody (Ab)-based proteomics play a very important role in biomarker discovery and validation, facilitating the high-throughput evaluation of candidate markers.

An important aspect in the validation of biomarkers and/or targets discovered in such a heterogeneous source of proteins as blood is their adequate biological validation through the understanding of their exact role in relevant pathophysiological processes. In this respect, proteomics technologies enabling pathway analysis, such as mass cytometry, bring great hope for future clinical applications.

Ab-based technologies remain the main solution to address this challenge since they reach higher sensitivity. Because Ab-related function by binding specific Antigens (Ags), attempts to identify Ab biomarkers have so far involved using Ags to capture Abs that are overproduced in disease.

Along with canonical Abs, some of the families proven to occur are Abs possessing with catalytic (proteolytic) activity (catAbs or abzymes) and thus to belong to Abs with a feature of functionality! In this context, Abs against myelin basic protein/MBP and Cardiac Myosin (CM) endowing with proteolytic activity (Ab-proteases with functionality) are of great value to monitor autoimmune demyelination and/or Autoimmune Myocarditis (AIM) to illustrate the evolution of Multiple Sclerosis (MS) and myocardial autoimmunity conditions, respectively.

Anti-MBP autoAbs from MS and AIM patients exhibit specific proteolytic cleavage of MBP and CM, respectively, which, in turn, markedly differed between: (i) MS and AIM patients and healthy controls; (ii) different clinical MS and/or AIM courses; (iii) EDSS scales of demyelination and cardiac autoimmunity scores, on to correlate with the disability of MS and/or AIM patients to predict the transformation prior to changes of the clinical courses.

Ab-mediated proteolysis of MBP and CM was shown to be sequence-specific whilst demonstrating sites of preferential proteolysis to be located within the immunodominant regions of MBP and CM, respectively.

The activity of MBP- and CM-targeted Ab-proteases was first registered at the subclinical stages 1-3 years prior to the clinical stages of the disorders (preillness conditions) of both MS and AIM. About 15-25% of the direct MS- and AIM-related relatives were seropositive for low-active Ab-proteases from which 22-28% of the seropositive relatives established were being monitored for 2-3 years whilst demonstrating a stable growth of the Ab-associated proteolytic activity. Moreover, some of the low-active Ab-proteases in the compromized persons at MS- and/or AIM-related risks (at the subclinical stages), and primary clinical and MRT manifestations observed were coincided with the activity to have its mid-level reached.

As we might see, Abs can assist in the determination of staging, grading, and primary therapy selection, and after diagnosis, for monitoring therapy, additional therapy selection, or monitoring recurrent diseases. In this sense, the activity of Ab-proteases in combination with the sequence-specificity would confirm a high subclinical and predictive value of the tools as applicable for personalized monitoring protocols.

And the primary translational potential of this knowledge being rooted in the rational design of the new Ab-driven therapeutics and based on principles of natural and artificial biocatalysts, has started up exploiting the role of the key pathways in influencing disease. And improvements in biodesign-inspired engineering technologies, combined with bioinformatics-driven algorithms suggesting that catalytic Abs (Ab-proteases, in this cases) being natural or design-driven ones, play a valuable role in the living systems, have opened the way to new applications for those proteins as translational tools.

The last years have seen a major upturn in the fortune of therapeutic Abs, approved for clinical use. Ab-based therapeutics have entered the center stage of drug discovery as a result of a major shift in focus of many biopharma companies. This success, for instance, can be related to the engineering of mAbs into chimeric Abs, or humanized ones, which have had a major effect on immunogenicity, effector function and half-life. Emerging have created a vast range of novel, Ab-based therapeutics, which specifically target biomarkers of disease in this sense, Ab-proteases can be programmed and re-programmed to suit the needs of the body metabolism or could be designed for the development of principally new catalysts with no natural counterparts. The latter would suit the needs of the body metabolism or could be designed for the development of principally new catalysts with no natural counterparts So, Ab-protease-driven engineering would offer the ability to enhance or alter their sequence-specific activity to expand the clinical utility of the absolutely new tools.

In this context, immunotherapy is emerging as a promising route towards the Ab-mediated selective targeting, and future developments in intracellular Ab technology may enhance the therapeutic potential of such Ab-derived therapies. So, targeted Ab-mediated proteolysis could be applied to isolate from Ig molecules catalytic domains directed against immunogenic autoepitopes or domains containing segments to exert targeted proteolytic activity.

Meanwhile, the next important step in the direction of the innovations-based approach should be their early adoption in clinics for future medical interventions! And we have made the first step in this direction to improve the management of chronic autoimmune conditions.

The field of therapeutic Abs has become a dominant force in the therapeutics market. In the future, studies evaluating synergistic effects of catalytic Abs will greatly benefit the further development of Ab therapeutics. And we might believe and expect that autoimmune diseases are promisingly suited and evidence-based models to support the above-mentioned strategy because of the rapidly expanding Hi-Tech innovations and design-inspired translational resources, including ABZYMES technologies and the development of biomarkers and the potential modifying treatments.

Furthermore, the identification of novel biomarkers may improve the efficacy and specificity of Ab-based therapy for human diseases.

Audience Take Away Notes

- Only positions and vacancies of the next step generation in the faculty niches, applied and translational research and applications
- For teaching using diagnoctis and predictive OMICS-driven technologies, including PCR, NGS, GWAS testing, immunochemistry and ELISA
- Directly. Ab proteases would depict design-driven innovative approaches aiming at the monitoring and management of multiple sclerosis patients and pre-illness persons-at-risk
- It 100% improves the accuracy of a design, or provide new information to assist in a design problem

Biography

Sergey Suchkov was born in the City of Astrakhan, Russia, in a family of dynasty medical doctors. In 1980, graduated from Astrakhan State Medical University and was awarded with MD. In 1985, Suchkov maintained his PhD as a PhD student of the I.M. Sechenov Moscow Medical Academy and Institute of Medical Enzymology. In 2001, Suchkov maintained his Doctor Degree at the National Institute of Immunology, Russia. From 1989 through 1995, Dr. Suchkov was being a Head of the Lab of Clinical Immunology, Helmholtz Eye Research Institute in Moscow. From 1995 through 2004 - a Chair of the Dept for Clinical Immunology, Moscow Clinical Research Institute (MONIKI). In 1993-1996, Dr. Suchkov was a Secretary-in-Chief of the Editorial Board, Biomedical Science, an international journal published jointly by the USSR Academy of Sciences and the Royal Society of Chemistry, UK. At present, Dr Sergey Suchkov, MD, PhD, is: Professor and Chair, Dept for Personalized Medicine, Precision Nutriciology and Biodesign, the Institute for Biotech & Global Medicine of RosBioTech, Moscow, Russia. Professor, Dept for Clinical Immunology, A.I. Evdokimov Moscow State University of Medical and Dentistry, Moscow, Russia Member, New York Academy of Sciences, USA. Secretary General, United Cultural Convention (UCC), Cambridge, UK. Dr. Suchkov is a member of the: American Chemical Society (ACS), USA; American Heart Association (AHA), USA; European Association for Medical Education (AMEE), Dundee, UK; EPMA (European Association for Predictive, Preventive and Personalized Medicine), Brussels, EU; ARVO (American Association for Research in Vision and Ophthalmology); ISER (International Society for Eye Research); Personalized Medicine Coalition (PMC), Washington, DC, USA.



Sevda Mozaffari*, Dr. Gholamreza Heydari

Tobacco prevention and control research Center, National research institute of tuberculosis and lung diseases, Shahid Beheshti university of medical sciences, Tehran, Iran

Evaluation of the effects of PAKDAM, an invented device to get nitrous oxide and oxygen, in the consumers : A report of pilot study in Tehran 2022

Many studies showed that the combination of Nitrous Oxide (N_2O) and Oxygen (O_2) led to a reduction pain, greater respiration. About a decade the device, which was called PAKDAM (means clean inspiration) was invented in Iran and has been used in some cafe to prepare N_2O and O_2 as a new instrument instead of water pipe. The goal of this study was to evaluate the effects of Pakdam and investigating its short and midterm side effects in users. The Method was a case-control study which was done between September 2021 and March 2022. Subjects were divided into two groups: consumers (case) and non-consumers (control). The result showed that blood oxygen level and FEV1 / FVC ratio were higher in people using Pakdam and the amount of exhaled carbon monoxide was lower. This condition was more common in smokers and less in non-smokers. It can be considered that the desired effects of the device were greater for smokers

Audience Take Away Notes

- It will possible to use as an alternative device to Water pipe in some public places were serving it
- Oxygen therapy is offered as a method of respiratory care when there is a respiratory problem as well as Oxygen therapy ensures better and more active function
- In this study was the possibility of replacing this device with Water pipe according to having the same shape and psychologically condition and does not have the harmful effects of tobacco consumption, it may investigate in a new study to be used as an alternative device to Water pipe in some public places were serving it
- According to the demand for Water pipe smoking is increasing, and even given the implementation of tobacco control programs in many countries, this social and health problem still exists. Therefore, it is very critical to find a solution that can be a healthy alternative behavior to reduce or eliminate hookah smoking
- It is possible to see the favorable effects of using Pakdam device on people. However, according to the sample size in the pilot study and to generalize the results, further studies should be conducted in larger sample size with different demographic variables
- In this study, it was found that blood oxygen level and FEV1 / FVC ratio were higher in people using Pakdam and the amount of exhaled carbon monoxide was lower. This condition was more common in smokers and less common in non-smokers. It can be considered that the desired effects of the device were greater for smokers. Using this device, instead of releasing carbon dioxide and tobacco into the air, excess oxygen is released into the air, creating clean air in these places

Biography

Miss Mozaffari studied Hydraulic Structure at the Tabriz University, due to her father's invention (Pakdam device), She then joined the research group of Prof. Gholamreza Heydari at the National research institute of tuberculosis and lung diseases, Shahid Beheshti university of medical sciences.



Shawn Gouws*, Jason Mackay
Department of Chemistry, Nelson Mandela University, Gqeberha, South Africa

Characterization of Ir-based catalysts for PEM electrolyser

Large quantities of industrial hydrogen are produced from fossil fuels, which leads to a large carbon footprint that slowly destroys our planet. Therefore, a need arises to reduce the carbon footprint in numerous industrial processes such as methanation, methanol, and ammonia. One possible route my group is investigating is using proton exchange membrane water electrolysers to produce green hydrogen for these industrial processes. We investigate Proton Exchange Membranes (PEM) because of the abundant Platinum Group Metals (PGM) mined in South Africa. Although PEM has several advantages, such as high current densities, it pairs well with other renewable energies, such as solar or wind, low gas permeability and faster hydrogen production with minimum environmental waste. A disadvantage, however, is the capex expense of utilising PGMs such as iridium and platinum—as well as acid corrosion components.

Our research shows for the preliminary results for IrM (M=Ru, Ti, and Au) bimetallic mixtures that similar robustnescould be obtained for iridium only as the oxygen evolution reaction catalysts. This paper will discuss the preliminary results through material characterisation XRD, XRF and TEM analysis, cyclic voltammetry, linear voltammetry and chronopotentiometry.

Current research involves manufacturing the membrane electrode assemblies and testing these in PEM water electrolysers for durability and robustness. To do this, a small test rig will be built and commissioned with solar PV cells to produce green hydrogen from renewable energy resources.

Keywords: PEMWE, Water Electrolysis, OER.

Audience Take Away Notes

- Bimetal complexes or metal mixtures with Ir could reduce capital costs
- Green hydrogen is needed to reduce the carbon footprint of industrial processes
- Electrochemistry is key to analyzing the electrocatalyst's characterisation of this catalyst
- More research is needed to overcome the demand for producing green hydrogen

Biography

Dr. Shawn Gouws studied Chemistry at the Port Elizabeth Technikon (now Nelson Mandela University), Gqeberha, South Africa and graduated from DTech in 1999. He joined LEORR, Grenoble, France, in 2000 to complete a one-year post-doctoral fellowship under Dr. Sylvie Chardon-Noblat. He then joined the late Prof Ben Zeelie's group at InnoVenton, Nelson Mandela University, researching process chemistry and electrocatalysts. He has published 15 articles in SCI journals, filled four patent applications, and written one book chapter. His research interest is electrocatalysis for PEM water electrolysers to produce green hydrogen.



Dr. Shree Niwas Chaturvedi[1]*, Ashok Poddar[2]

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Water splitting technology for efficient thermal energy conversion process

This abstract presents an invention patented by Government of India. This invention utilizes water (steam) splitting/water gas shift process which converts gaseous fuel mixture being produced by the burning of carbonaceous solid fuel, into progressive generation/production of hydrogen in fuel mixture and continuous combustion of hydrogen along with other combustible components and atmospheric gases. The temperature produced during the combustion is 1600 ^{0}C - 1900 ^{0}C. The most important part of the invention is that it does not use any catalyst for hydrogen production. Thus the invention can be utilised as next generation most efficient Thermal Energy Generation/Producing Equipment/Process/ System at very low cost.

Audience Take Away Notes

- The audience will learn about new technology of pollution free low cost high energy production system
- Since the paper is related to high energy production system at very low cost, it will help only those organizations which use energy at high level
- Other faculty could use this research to expand their research or teaching
- This provides a practical solution to a problem that could simplify or make a designer's job more efficient
- It improves the accuracy of a design, or provide new information to assist in a design problem

Biography

Shree Niwas Chaturvedi has immediately after earning his Ph.D in Chemistry (Nuclear and Radiochemistry) from Banaras Hindu University, Varanasi, India, in the year 2000, Dr. Chaturvedi founded 'Centre for Aptitude Analysis & Talent Search' which is also known as 'the EXPLORER'. Dr. Chaturvedi works with a philosophy that every child has unique talent which needs to be explored based on their aptitude. The institute has produced scores of students successful in different walks of life. Also, he is scientific adviser to Ganesh Engineering Works, Buxar.



Silvia E. Asis*

Universidad de Buenos Aires, Facultad de Farmacia & Bioquimica. Departamento de Ciencias Quimicas/ Junin 965, Ciudad Autonoma de Buenos Aires, Argentina

Synthetic quinolines and related heterocycles in the discovery of new agents against M. tuberculosis and NTM

Tuberculosis (TB), caused by the bacteria Mycobacterium Tuberculosis (Mtb), is still one of the world's greatest threats. Ending the TB epidemic by 2030 is among the health aims of the United Nations Sustainable Development Goals (SDGs). Moreover, the incidence and number of deaths from Nontuberculous Mycobacterial Disease (NTM) have been steadily increasing globally and these mycobacteria have become extremely resistant to antibiotics and are easily dispersed by migration and climate change. Our research group has been developing quinoline derivatives with anti-TB activity for more than fifteen years. Although initially targeted as antimalarial agents, the design was focused on anti-TB activity, inspired by natural active alkaloids. The discovery of bedaquiline and its approval by the FDA was the driving force to design new 2,4-diarylquinolines as well as polycyclic and fused quinolines. To design new antituberculosis agents with a quinoline structure, our group developed Three-Dimensional Structure-Activity Relationship (3D-QSAR) models, based on Comparative Molecular Field Analysis (CoMFA) and Comparative Molecular Similarity Index Analysis (CoMSIA). These models were used to find the key structural features and design fifteen new compounds prepared via the MW-assisted Friedlander reaction in good yields, with inhibition growth activity against M. tuberculosis. In addition, was explored the potential application of the designed compounds as growth inhibitors on resistant M. tuberculosis culture, as well as against non-tuberculosis culture among them M. avium and M. abscessus.

Audience Take Away Notes

- Other faculty could use this research to expand their research or teaching
- It improves the accuracy of a design, or provide new information to assist in a design problem
- Other benefits
    - Knowing about Tuberculosis and Nontuberculous Mycobacterial disease (NTM), discovery of hit anti TB compounds

Biography of Silvia E. Asis

Dr. Asis studied Chemistry at Universidad Nacional de Córdoba, Argentina and graduated as MS in 1988. She received her PhD degree in 2001 at Universidad de Buenos Aires. She has extensive experience in teaching organic chemistry and has obtained the position of an Assistant Professor in 2017. She has been leading her line of research for many years and has published 29 papers in the medicinal chemistry area.



Christopher L. Cioffi[1], Arun Raja[1], Parthasarathy Muthuraman[1], Aravindan Jayaraman[1], Srinivasan Jayakumar[1]*, Andras Varadi[2], Boglarka Racz[2], Konstantin Petrukhin[2]

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Identification of transthyretin tetramer kinetic stabilizers to inhibit retinol-dependent RBP4-TTR interaction: Novel therapeutics for macular degeneration and transthyretin amyloidosis

The interaction between Retinol-Binding Protein 4 (RBP4) and Transthyretin (TTR) is implicated in the pathogenesis of diseases such as macular degeneration and transthyretin amyloidosis. Our study identifies novel kinetic stabilizers of the TTR tetramer, offering a therapeutic strategy to inhibit this critical interaction. Through a robust screening of chemical libraries, we isolated compounds that effectively stabilize TTR tetramers. These stabilizers were shown to disrupt the RBP4-TTR interaction, a novel approach in managing these diseases. Our analyses confirm the efficacy of these stabilizers in reducing TTR aggregation. This research opens avenues for developing treatments for macular degeneration, transthyretin amyloidosis, and their related comorbidities, potentially impacting patient care for these age-related conditions.

Introduction to TTR Amyloidosis and Macular Degeneration:

- Overview of diseases and their impact.
- Role of RBP4-TTR interaction in disease pathogenesis.

Objective of the Study:

- Aim to identify TTR tetramer kinetic stabilizers.
- Potential impact on disease treatment.

Methodology:

- Description of chemical library screening for stabilizers.
- Biochemical assays and cellular models used.

Key Findings:

- Identification of compounds that stabilize TTR tetramers.
- Efficacy in disrupting RBP4-TTR interaction.

Analysis and Interpretation:

- Discussion on how stabilizers reduce amyloid fibril formation.
- Insights into the molecular mechanisms involved.

Implications for Treatment:

- Potential for these compounds in treating TTR amyloidosis and macular degeneration.
- Discussion of how these findings could influence future therapeutic strategies.

Concluding Remarks:

- Summary of the study's significance.
- Future research directions and potential clinical applications.

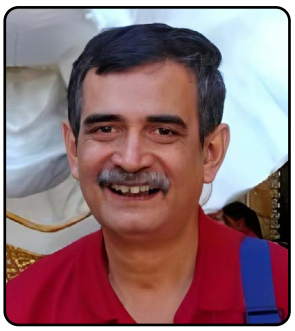
Audience Take Away Notes

- **Understanding of TTR Amyloidosis and Macular Degeneration:** The audience will gain a comprehensive overview of these diseases, their impact on health, and the role of the RBP4-TTR interaction in their pathogenesis
- **Innovative Therapeutic Approaches:** Insight into the identification and role of Transthyretin (TTR) tetramer kinetic stabilizers in disrupting RBP4-TTR interactions, a novel therapeutic strategy
- **Scientific Methodology and Discovery:** Insights into the methodology used for identifying these stabilizers, including chemical screening and various assays
- **Clinical Implications:** The efficacy and potential therapeutic impact of these stabilizers in treating TTR amyloidosis and macular degeneration
- **Future Research Directions:** Future directions for research and potential clinical applications of these findings.
- **Applications of the learnings:**
    a. Audience members involved in research or clinical practice can apply this knowledge to gain insights into new therapeutic strategies for managing TTR amyloidosis and macular degeneration, enriching their understanding of potential future treatments
    b. Audiences involved in pharmaceuticals or drug development can use this information to explore new avenues for medication development
    c. Educators and students can incorporate these findings into academic discussions, enhancing the understanding of disease mechanisms and treatment strategies
- **Professional Benefits:**
    1. The outcomes of this research have the potential to guide clinical decisions and treatment strategies for healthcare professionals managing TTR amyloidosis and macular degeneration
    2. Researchers may leverage these discoveries as a foundation for additional investigations, possibly paving the way for innovative treatment approaches
- **Expansion Research and Teaching:**
    1. Other faculty members could integrate these findings into their research, exploring related compounds or mechanisms
    2. The information can be used in academic settings, enriching teaching curriculum, especially in fields related to biochemistry, pharmacology, and ophthalmology
- **Practical Approach for Designers:**
    1. This research offers a foundation for developing new drugs, aiding pharmaceutical designers in creating more effective treatments
    2. The identification of specific compounds provides a direct pathway for drug development, potentially streamlining the process
- **Enhancing Design Precision and Addressing Issues:** This research provides new information that could be crucial in resolving challenges as well as designing more targeted and effective therapeutic interventions for TTR amyloidosis and macular degeneration

- Other benefits
    - Encourages interdisciplinary collaboration between researchers, clinicians, and pharmaceutical companies
    - Potentially stimulating further research, leading to breakthroughs in other age-related diseases
    - Contributes to a broader understanding of protein interactions and their implications in disease, which can be applied to various fields of biomedical research

Biography

Dr. Srinivasan Jayakumar is an accomplished Postdoctoral Research Associate currently affiliated with the Rensselaer Polytechnic Institute in New York, USA. He specializes in Synthetic Organic and Medicinal Chemistry, bringing over eight years of detailed research experience which includes five years of Industrial experience at Syngene International Pvt Ltd, India. Dr. Jayakumar's educational background includes a Ph.D. in Organic Chemistry from National Tsing Hua University, Taiwan, and a Master's in chemistry from Guru Nanak College, University of Madras, India. In 2020, he transitioned to the U.S., undertaking a postdoctoral research position at Albany College of Pharmacy and Health Sciences, NY, and is currently engaged with Rensselaer Polytechnic Institute in Troy, NY. Dr. Jayakumar's notable research focuses on developing GlyT2 inhibitors for the treatment of neuropathic pain and RBP4 antagonists for the treatment of age-related macular degeneration, Transthyretin Amyloidosis, and their Common Age-related comorbidities. In addition to his research work, Dr. Jayakumar actively contributes to the scientific community. He serves on the editorial boards of several international chemistry journals and has a strong track record as a journal reviewer. His publications span a range of topics in medicinal and synthetic organic chemistry, reflecting his broad expertise and commitment to advancing the field.



S. K. Bandyopadhyay
Retired Scientist, Variable Energy Cyclotron Centre, India

Multifunctional nanostructured materials: A new dimension in energy storage materials

Multifunctional materials are of today's quest. Miniaturization, i.e. development of these materials in the form of nanomaterials is of primary need considering their application in devices. Moreover, if these are obtained in nanostructured form, they can bring wonders.

Recently, a we have adopted for developing multiferroic $BiFeO_3$ (BFO) with simultaneous antiferromagnetic, ferroelectric & ferroelastic behaviour in form of nanostructures like nanorods, nanowire etc. by employing Anodised Alumina (AAO) template with various pore sizes from 20nm with solution route followed by controlled vacuum filtration and sintering. Diameters of nanorods are in the range of 20-100 nm as observed by FESEM. Capacitance assayed by Cyclic Voltammetry (CV) and charge discharge processes reveals a very high value of specific capacitance of 450F/gm. Capacitance has been estimated by extrapolating the charge collected at the electrode to that at scanning rate of infinity which is relevant for the charge collected at the nanorods protruding out of the template. Charging and discharging times are quite constant over a large number of cycles. This large value of specific capacitance can be attributed to the nanostructure form of BFO nanorod. The high value of specific capacitance of BFO nanorods brings forth its use as electrode in storage energy devices.

Biography

Dr. Sujit Kumar Bandyopadhyay, Emeritus Fellow, Meghnad Saha Institute of Technology (from 2017 to 2020) and Institute of Engineering and Management (2020-2021). Ex-Head, Material Science Studies Division, Scientific Officer (H)+ and Professor, Homi Bhabha National Institute, Variable Energy Cyclotron Centre (VECC), Dept. of Atomic Energy, Govt. of India. (Retired on Superannuation on 30th September, 2015). **Academic and Professional Background:** 1978: Joined Chemical Engg. Division, Bhabha Atomic Research Centre as Scientific Officer. 1982: Joined Variable Energy Cyclotrn Centre, as Scientific Officer. 1998: PhD (Physics) from Jadavpur University. Title of Thesis: Charged Particle Irradiation Studies on Copper Oxide Superconductors. Post Doctoral fellow: Atomic Institute of Austrian Universities, Vienna, 2000, in the field of Magnetisation studies of neutron irradiated HTSC superconductor single crystals. Professor, Homi Bhabha National Institute, deemed University since 2009. **Awards:** 1. National Science Talent Search (NSTS) Scholarship, 1971. 2. National Scholarship, Government of India, 1971. 3. A P J Abdul Kalam award for utstanding research. Current Areas of Interest: Multifunctional Materials in Nanostructured form and their application as energy storage material. A). Capacitance Studies on Multifunctional nanostructured materials with respect to their application as energy storage device. Publications: Journal papers & Articles in books: 86. Proceedings in National & International Conferences: 66. Author of e-book Charged Particle Irradiation Studies on Bismuth Based High Temperature Superconductors & MgB2; A Comparative Survey. Regular Reviewer in Science Direct journals like Materials Chemistry & Physics, Jl. Of alloys and compounds and Jl. Of Solid State Chemistry. Reviewer of Ph.D. Theses of various universities like Burdwan University, Tejpur University etc. Registered Guide for a) Jadavpur University and b) HBNI.



Theodosios Geo Douvropoulos
Hellenic Naval Academy/Physical Sciences Sector, Piraeus Greece

Resonant transport time in $Al_xGa_{1-x}As$/GaAs nanostructures and mass discontinuity: A semiclassical path integral approach

In the current work, we investigate the dependence of the carrier transport time in an AlGaAs/GaAs heterostructure on the carrier's effective mass discontinuity between the well and the barrier layer. The effective mass consists of a simple approximation to take into account the complexity of the carrier's interactions and treat the carrier as a free particle. The mass discontinuity is directly related to the mole fraction of x, where x represents the concentration of Al. A double barrier potential in the direction of vertical growth is assumed to be the one-dimensional model effective potential of the system. The resonant tunneling mechanism is activated when a bias is applied between the emitter and the collector, which are both heavily doped GaAs regions. We calculate the system's Green's function through semiclassical path integration and get the complex spectrum. The imaginary part of the spectrum is the width of the resonant state of the well, which is the inverse of the corresponding lifetime. The latter is assumed to be equal to the carrier transport time and is given through analytic relations depending on various parameters, including the mass discontinuity factor. Thus, charge transport can be significantly boosted and controlled by the resonant tunneling effect. Charge transport depends on many different physical parameters, such as the energy value, the dimensions of the heterostructure, the model encountered for the description of the effective potential on the growth direction, the carrier's effective mass, and others. Charge transport is maximized when the resonance conditions of the GaAs quasibound state well are met.

In our presentation, we will first briefly expand on the main characteristics of a generic potential modeling the heterostructure, consisting of a double barrier structure and a quantum well between them when a bias is applied. Next, we will present the path integral method and construct the system's fixed energy amplitude. The latter reveals the complex resonance positions calculated in the next section. We show how to calculate transport time as a function of the mass discontinuity between the AlGaAs and the GaAs regions, and other characteristics such as the barrier width and height and the applied bias.

Audience Take Away Notes

- Someone can actually apply the method described here, to realistic $Al_xGa_{1-x}As$/GaAs Nano-structures and calculate the time needed for resonant transport
- As mentioned in the abstract, this work connects the effective mass discontinuity with transport time. It offers physical insight to the definition of the effective mass and possible corrections based on experimentally observed time scales of the heterostructure. In addition someone can learn about path integrals and think about expanding his teaching by incorporating the method
- Since the findings of the current work come in analytic form, a designer may vary Aluminum's concentration to reach the desired transport time with high accuracy
- **New information:** Transport time proves to act somehow as the nanostructure's identity

Biography

Dr. Theodosios Geo Douvropoulos studied Physics at Patra University, Greece (1996). He then joined the research group of Prof. C.A. Nicolaides at the National Hellenic Research Foundation (Theoretical Physics and Chemistry Institute), where he received a Master's degree in Physics (2001) and his Ph.D. degree (2005) in Quantum Dynamics. His main research activity is about the quantum evolution of low-dimensional physical and chemical systems. He has published more than 20 research articles and has obtained the position of lecturer at the Hellenic Naval Academy of Greece since November 2022.



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Chemically induced proximity regulates protein function and degradation

Proximity, or the physical closeness of molecules, is a pervasive regulatory mechanism in biology. To understand the role of proximity in biologic mechanisms, Chemical Inducers of Proximity (CIPs) or Chemical Inducers of Dimerization (CIDs) were developed; these bifunctional small molecules bring two proteins in close proximity and subsequently enable precise temporal control of various cellular processes, such as cell signaling cascades, protein-protein interactions, cellular cargo transport, and genome editing. In this abstract, we are going to present three major types of CIP technologies our group have developed in recent years: i) nanobody-based CIP, or SNACIP, for regulation of intracellular protein functions (Nat. Commun. 2023); ii) autophagy-targeting nanobody chimera, or ATNC, for regulation of protein degradation (J. Am. Chem. Soc. 2023); and iii) photo-responsive CIPs, or chemo-optogenetic dimerization, for spatiotemporal control of protein functions by light (Angew. Chem. Int. Ed. 2018/ 2018). The first part is small molecule-nanobody conjugate induced proximity, or SNACIP, which was an integrated technology by combing 3 recent advancements from different fields, namely, i) CIP, ii) chemical nanobody engineering, and iii) cyclic arginine-rich peptide-based non-endocytic delivery system. As a nanobody-based CIP, SNACIP allows modulation of unligandable targets and endogenous Intrinsically Disordered Proteins (IDPs), which represent challenging targets for traditional CIP/CID tools. The second part is ANTC technology, which uses nanobody-fused chimeras that recruit proteins to autophagy degradation pathway. Therefore, ATNC is able to degrade unligandable and undruggable proteins. The third part is chemo-optogenetic dimerization approaches which were developed by combing CIP concept and optogenetics. Chemo-optogenetic tools can be considered as a Chemistry version of optogenetics, exhibiting unique features and advantages. These examples showcased the important roles and great potentials of chemical induced proximity-based technologies for biology and medicine applications.

Audience Take Away Notes

- In this talk, Prof. Xi Chen will present frontier chemically induced proximity-based tools for control of protein function, protein degradation and to regulate cellular activities by light. These tools will provide useful instructions for researchers in the related fields new means to study cellular functions and to degrade proteins for biological and biomedical purposes. The chemo-optogenetic dimerization approaches also offer photo-triggered dimerization tools for perturbation of cellular activities by light in a spatial and temporal manner

Biography

Professor Xi Chen received his Bachelor's degree in Chemistry at the Sichuan University, and graduated as MS at the National University of Singapore. He received a Ph.D. degree in Protein Chemistry under the supervision of Prof. Tanja Weil at Ulm University in 2012. Then he conducted postdoc research at the Max Planck Institute of Molecular Physiology and spent another 1.5 years as a senior scientist at Princeton University before joining Harbin Institute of Technology as a Principal Investigator. Prof. Xi Chen has published around 30 SCI journals, and his research interest is CIP-based chemical biology tools and their biological applications.



Xibo Yan
School of Chemical Engineering and Technology, Tianjin University, Tianjin, China

The construction and application of photoactivated polymer colloidal motors

Artificial colloidal motors are self-propelled tiny machines that mainly rely on chemically or physically responsive components working as kinetic systems for converting external energy into mechanical motion. This stimulus-responsive self-propelled locomotion would effectively strengthen the material performance in various applications, including drug delivery, sensing, imaging and environmental remediation. In the last decades, considerable efforts have been made to develop advanced kinetic systems of colloidal motors for programmable manipulation and precise modulation of mechanical work. In the presentation, we will introduce the design and development of photoactivated polymer colloidal motors, which would carry out autonomous movement powered by photo-responsive energy conversion (e.g. photocatalytic reaction, photothermal conversion, photoisomerization, etc.) within polymer components in response to photoirradiation. Thanks to the great flexibility of polymers in structures, properties and functions, the polymer-based colloidal motors allow on-demand programming various energy-converting behaviors (e.g. mono-mode, multimode sequential, multimode synergistic, etc.) within the materials, regulating the motile features of the colloidal motors for various sophisticated applications. In contrast to conventional heavy metal-made colloidal motors, these biocompatible polymer ones show great advantages in biomedical applications. The non-invasive and penetrative light-driven self-propelled delivery would endow the motors with high permeability against biological barriers in the solid tumor microenvironment to promote tumor accumulation, deep tumor penetration and cellular uptake, improving the delivery of nanomedicines. Besides, the light-driven energy conversion within the materials would also modulate the physiological microenvironment of the solid tumor (e.g. hypoxia, interstitial fluid pressure, etc.) for facilitating the antitumor therapy. Combining all these benefits, the photoactivated polymer colloidal motors would significantly enhance the antitumor efficacy.

Audience Take Away Notes

- Recent progress in photoactivated polymer colloidal motors
- The motile mechanisms of polymer colloidal motors in response to photoirradiation
- Potential applications of photoactivated polymer colloidal motors

Biography

Dr. Xibo Yan received his B.E. degree from Tianjin University and his M.S. degree from Nankai University. He completed his Ph.D. research under the guidance of Prof. Etienne Fleury from INSA de Lyon in 2015. After working as a post-doctoral researcher at Laboratoire Ingenierie des Materiaux Polymeres (Lyon) with Dr. François Ganachaud and Dr. Julien Bernard for three years, he began his independent career as an associate professor at Tianjin University in 2019. He has published more than 30 research articles in SCI journals. His research interests include intelligent polymeric nanomaterials, polymer self-assembly and biomacromolecules.



Xin Cui*, Xue Xu
Department of Chemistry, Mississippi State University, Mississippi, United States

Selective and sustainable catalysis for transforming C-H bonds

The development of green approaches to access new functional molecules has been impacting and improving the quality of lives. Processes with the best possible step and atom economy have been a preeminent goal of synthetic chemistry. Seeking new reactivity and selectivity in catalysis provides enormous opportunities for the construction of molecular complexity. Research in our laboratory focuses on developing next-generation inorganic and organometallic catalysts, and their applications in synthetic and medicinal chemistry. We are particularly interested in organometallic and mechanistic study-guided development of new patterns of selectivities for bond activation, bond formation, and tandem catalysis. Among ongoing directions, our group has been developing ruthenium(II)-catalyzed C–H functionalization processes as mechanistically unique and operationally practical tools for the stereoselective functionalization of various sites of arenes and alkenes. With the specific directions, we aim to gain new understandings and enrich selective and sustainable access to new molecules that have close relevance to bioactive compounds, chiral organic materials, synthetic building blocks, and future ligand toolboxes for catalysis.

Audience Take Away Note

- The audience will learn about recent development in sustainable methods for converting C-H bonds to functional molecules
- The practical, energy and material-saving design of the catalytic processes would encourage industry applications for drug molecule synthesis
- The application of co-catalysis for this development in controlling the stereoselectivity and reactivity for C-H functionalization would inspire the design of new green synthesis with minimum energy consumption and waste generation

Biography

Xin Cui received his B.S. in chemistry and Ph.D. from the University of Science and Technology of China. He received his postdoctoral training at the University of South Florida. After a one-year as an assistant professor at Baruch College at the City University of New York, he joined the Department of Chemistry at Mississippi State University in 2016. He is currently an Associate Professor of Organic, Organometallic and Inorganic Chemistry.



Merzouk Zatout
Kasdi Merbah University, BP 511. 30 000 Ouargla, Algeria

Modeling of water flooding effects during enhanced oil recovery

Water flooding secondary oil recovery method was adapted to enhance oil production from the Algerian X-field by maintaining reservoir pressure and replacing the recovered oil quantities. However, this operation has some negative effects on the reservoir rock and the production facilities. Indeed, several salts, including halite, anhydrite, calcite, barite, and celestine, are deposited in the rock reservoir, on the downhole completion equipment, along the tubing, and in the surface equipment such as wellheads, separators, and pipelines. On the other hand, the end of the diagenetic sequence for the reservoir sandstone marked by the bearing of the late anhydrite cement and iron cements such as pyrite and goethite. To understand the formation of these late diagenetic cements and salts observed after water injection, and the factors involved, a geochemical simulation of the individual/combined effects of Cambrian oil brine and Albian injection water was carried out. The PHREEQC software has been used with two different thermodynamic databases Pitzer.dat and llnl.dat. The Pitzer database is suitable for highly concentrated waters (brines) and tested for high pressure and temperature brines. The llnl.dat database is dedicated for high pressure and high temperature. It gave also good results, especially for speciation determination. Thus, the combination and comparison of these two databases performed to discuss the modelled results. The results obtained by the PHREEQC simulation perfectly reproduced the observations made. Indeed, the origin of the late diagenetic iron cement crystallized because of the supersaturation of the oil brine in pyrite, hematite and goethite during its installation in the Cambrian HMD trap after the oil secondary migration. In addition, interactions between sulphate-rich Albian water and Cambrian oil brine containing barium, calcium and strontium explain the precipitation of anhydrite, calcite, barite and celestine. The high concentration of sodium and chlorine in the oil brine, and the high temperature along the hydrocarbon production pathway explain the precipitation of halite throughout. This study shows that it is advantageous to simulate the water flooding operation with the starting water flooding and reservoir brine ionic compositions to predict the possible salts that will precipitate. Thus, many undesired solids can be avoided by selecting the most compatible waters and specific inhibitors for salts likely to crystallize.

Audience Take Away Notes

- From the presentation, industrialists operating in the oil and gas field will understand the importance of chemical interactions between injection fluids and reservoir effluents
- The simulation presented is only the beginning to perfect the model of the effects caused by the exercise of secondary recovery with the injection of water
- Certain minerals are not yet supported by known thermodynamic databases, a research work is fully opening up for academicians

Biography

Zatout Merzouk graduated as a geologist engineer in geological exploration at the Algerian Petroleum Institute in 1995. After 12 years as a petroleum geologist at the national petroleum company of Algeria (Sonatrach), he changed his employer to Ouargla University with a Master's degree diploma in geochemistry freshly obtained. Because of his strong background in petroleum geology, he assures all related courses to petroleum geology at the university. He graduated with a Ph.D. in geology in 2017. his field research is the geochemistry of brines. His finding confirms lithium occurrence in Saharan chotts and highlights the effectiveness of their mining potential.



Zhongyue Zhou[1]*, Linyu Zhu[1], Cunhao Cui[2], Fei Qi[1]

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[2]State Key Laboratory of Physical Chemistry of Solid Surfaces, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, Fujian, China

Thermochemical conversion of biomass: Probing oligomeric intermediates with online high-resolution mass spectrometry

Liquid-phase heterogeneous catalysis reactions are fundamentally important in fine chemicals, pharmaceuticals, energy conversion, and material synthesis. Catalytic conversion of biomass in liquid-phase is a typical one, involving solid catalysts, high temperature, high pressure, and complex products distribution. Intermediates are important fulcrum in the reaction network and hold the key to decipher the mechanisms involved in heterogeneous catalysis, but the measurement of such intermediates under operando conditions is challenging. In this presentation, we will introduce a versatile and efficient technique, named Reactor-Integrated Electrospray Ionization Mass Spectrometry (R-ESI MS), for operando probing intermediates in heterogeneous catalytic conversion of biomass conducted at high-pressure and liquid-phase conditions. Compared with traditional cook-and-look methods based on chromatography, the technique of R-ESI MS does not need any sample collection, pretreatment, transmission, and chromatographic separation steps, mitigating any risk of sample loss during sampling handling. It holds the unique advantage in direct and real-time measurement of products, especially heavy intermediates, under harsh reaction conditions. Furthermore, this methodology is developed on a commercial MS platform, and no specialized equipment is necessary, which is intended to provide a basis for wider applications in catalysis studies and may lead to more rapid discoveries of new catalysts.

Audience Take Away Notes

- Reactor-integrated electrospray ionization mass spectrometry for liquid-phase heterogeneous catalytic reactions
- Recent progress in mechanistic investigation of lignin degradation via probing oligomeric intermediates
- Potential of investigating heterogeneous catalytic reactions with online high-resolution mass spectrometry

Biography

Dr. Zhou received his Ph.D. degree from University of Science and Technology of China (USTC) in 2012. After three years postdoctoral fellowship at National Synchrotron Radiation Laboratory, USTC, he joined Shanghai Jiao Tong University. His research focuses on online mass spectrometry and fundamental chemistry in biomass conversion and solid propellants combustion. He has published more than 70 peer-reviewed papers. He serves as a Colloquium Co-Chair for the diagnostics colloquium of the 39th and 40th International Symposium on Combustion, Colloquium Co-Chair of the China National Symposium on Combustion, and review editors of Frontiers in energy research and Frontiers in Chemical Engineering.

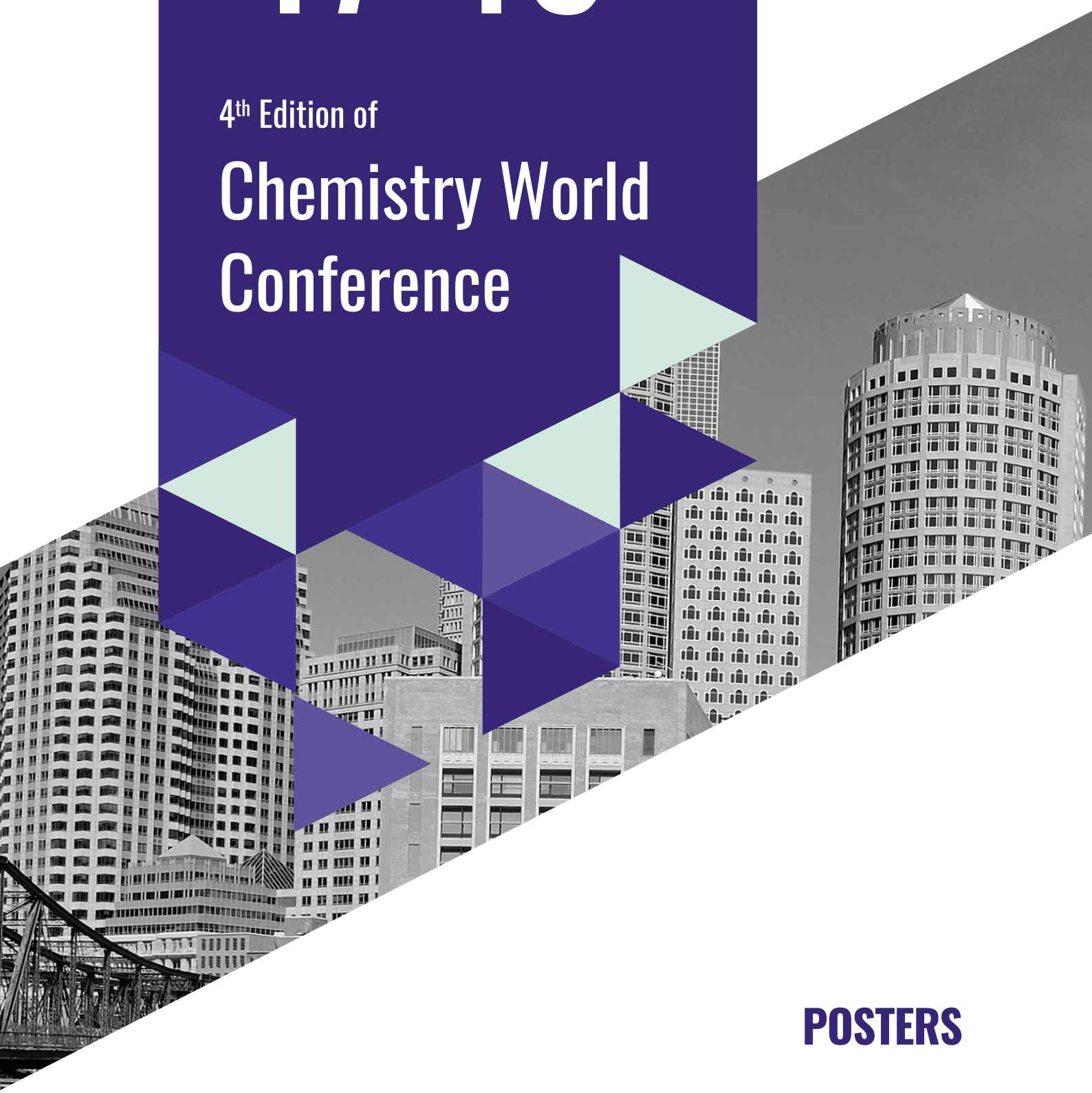
BOOK OF ABSTRACTS

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POSTERS



Julia A. Barbosa[1,2]*, Gabriel R. Schleder[1], Renato S. Lima[1,2]

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4.0 wearable plant sensor: Solving obstacles toward the long-term, accurate, and remote monitoring of water loss from plants under variable microclimate

Impedimetric wearable sensors are a promising strategy for determining the Loss of Water Content (LWC) from leaves because they can afford on-site and nondestructive quantification of cellular water from a single measurement. Because the water content is a key marker of leaf health, monitoring of the LWC can lend key insights into daily practice in precision agriculture, toxicity studies, and the development of agricultural inputs. Ongoing challenges with this monitoring are the on-leaf adhesion, compatibility, scalability, and reproducibility of the electrodes, especially when subjected to long-term measurements. This work introduces a set of sensing material, technological, and data processing solutions that overwhelm such obstacles. Mass-production-suitable electrodes consisting of stand-alone Ni films covered by gold obtained by well-established microfabrication methods enabled reproducible determination of the LWC from soy leaves with optimized sensibilities of 27.0 kΩ $\%^{-1}$. The electrodes operated through direct transfer of the conductive materials on hairy soy leaves using an ordinary adhesive tape. The freestanding design of the electrodes was further key to delivering high on-leaf adhesion and long-term compatibility. Their impedances remained unchanged under the action of wind at velocities of up to 2.00ms^{-1}, whereas X-ray nanoprobe fluorescence assays allowed us to confirm the sensor design compatibility by from the monitoring of the soy leaf health in an electrode-exposed area. The electrodes operated through direct transfer of the conductive materials on hairy soy leaves using an ordinary adhesive tape. We used a hand-held and low-power potentiostat with a wireless connection to a smartphone to determine the LWC over 24 h. Impressively, a machine-learning model was able to convert the sensing and reproducible responses in controlled conditions (30 and 20 °C) into a simple mathematical 3D equation that gauged the impairments on the water content with reduced root-mean-square errors (0.1% up to 0.3%). Next, analyses under The evaluation in a relevant environment with highly variable climatic conditions were performed to scrutinize the applicability of the sensor. The Ni films were covered by Au thin film (100 nm) led us to improve manufacturing, to avoiding problems such as oxidation of electrode over long-term monitoring (45 to 70 h) components and instability in electrical contact. Furthermore, Random-Forest was able to show that the importance of time variables has greater weight than temperature, humidity, and lower frequencies for predicting LWC. Remarkably, the A big data of impedances wereas converted into a low-dimensional and simple descriptor by the supervised Sure Independence Screening and Sparsifying Operator (SISSO) obtained a simple 2D equation to afford quantification of the LWC with a compromise between accuracy and the simplicity and speed of computation, dispensing temperature and moisture values as input data. The prediction accuracy boosted gradually along independent analyses, as expected from a sensor 4.0-based platform. These data results suggest the broad applicability of the platform by enabling direct determination of the LWC from leaves at variable climatic conditions. Overall, our findings may help to pave the way for translating sense–act technologies into practice toward the on-site and remote investigation of plant drought stress. These platforms can provide key information for aiding efficient data-driven management and guiding decision-making steps.

Audience Take Away Notes

- The public will be able to learn how to address common issues within the emerging field of wearable sensors in plants. This provides a practical solution with various proof of concepts, offering a platform that can be used to assist in precision agriculture, plant material toxicity studies, evaluation of new agricultural fertilizers and pesticides, effects of pathogens, or any other variable correlated with plant water content, in real-time and continuously for long periods
- Furthermore, the platform offers solutions for scalable manufacturing of wearable sensors in a simple and robust manner, including adhesion, biocompatibility with the plant, analytical sensitivity, low-noise, and electrical contact subject to fluctuations to sensing pads, and robustness in variable environments, subjected close to reality subject to excessive real climatic changes variables. It resolves and simplifies hardware implementations bysolely using machine learning, providing a simplified sample-to-answer platform
- Additionally, we provide a novel study using X-ray nanoprobes by Synchrotron radiation to evaluate the biocompatibility of the devices in the plant's physiological functions over a long period

Biography

Julia Barbosa is pursuing a Ph.D. at the Institute of Chemistry, University of Sao Paulo (Brazil) under the supervision of Dr. Renato S. Lima. The project has been is developed at the Brazilian Nanotechnology Laboratory of the Brazilian Center for Research in Energy and Materials, mainly focusing on microfabrication, capacitive electrochemistry, and machine learning for the development of a real-time plant health monitoring platform using wearable sensors. She holds a bachelor's degree in Chemistry education from the Federal University of São Carlos (Brazil), and during her undergraduate studies, she was involved in the development of methods in RP-HPLC methods and separation techniques for sample preparation of environmental samples.



M. Belen Gomez Mancebo*, Fernando Borlaf, Naiara B. Goikoetxea, Ana I. Sanchez Cabezudo, Ana I. Cardona, Rocio Fernandez Saavedra, Isabel Rucandio, Alberto J. Quejido

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Development of a methodology for ferrites evaluation by WDXRF

MFe_2O_4 (M: metal) (ferrites) are compounds widely employed in many industrial areas. The thermochemical water-splitting cycles, one of the most popular applications of these materials, have a significant potential to efficiently produce green hydrogen employing renewable energy resources. These thermochemical cycles can employ ferrites with spinel crystal structure. These cycles are known as ferrite cycles.

Spinel ferrites are considered appropriate candidates for two-step water splitting processes. In these cycles, the starting ferrite is reduced in the endothermic first step (activation), releasing oxygen, and then reacted with water (hydrolysis) to produce hydrogen and the pristine ferrite. These spinel ferrites are subsequently recycled to the first step and can be used in several hydrogen production cycles. This is a green hydrogen production process as it uses H_2O as a starting product and the final products obtained are H_2 and O_2.

In terms of cost, synthetic ferrites could be interesting candidates for scalable production. Different approaches of synthesis have been proposed, although co-precipitation method can be considered an easy and economical method for preparation of spinel ferrites. In this study, cobalt ferrite was synthetized by co-precipitation method using stoichiometric amounts of metal nitrates. To evaluate the performance of this method of synthesis is important the characterization of the as-prepared materials. Elemental characterization is mandatory, in this case, to determine the amount of each element in the final compound and Wavelength Dispersive X-ray Fluorescence (WDXRF) is an appropriated instrumentation for this evaluation. A methodology was developed and validated using WDXRF technique, for the evaluation of ferrites substituted with different metals (cobalt and nickel). An analysis of the sources of analytical uncertainty was also performed.

Acknowledgements:
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Audience Take Away Notes

- The public will be able to learn how to develop a simple method of quantitative analysis by WDXRF
- Additionally, it will be provided the methodology to perform a validation of the method
- Furthermore, this study supply a solution for studying the associated uncertainties of the whole process

Biography

Dr. M. Belen Gomez Mancebo studied Chemistry at the Complutense University, Madrid (Spain) and graduated in 1994. Then, she joined the research group of Prof. Carmen Camara at the department of Analytical Chemistry, at the Complutense University, Madrid (Spain). She received her PhD degree in 2002 at the same institution. After a three months postdoctoral fellowship supervised by Dr. R. Morabito at the National Agency for New Technology, Energy and The Environment (ENEA), Italy, she worked during three years in PPQF, Alcala de Henares University. Finally, she got a position as a senior scientist at CIEMAT, Madrid (Spain). She has published more than 40 research articles in SCI(E) journals.



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Radioactivity and heavy metal levels in mining areas of the state of Zacatecas, Mexico

Mining activities are prone to release toxic elements into soils through tailings, worthless ores, and subsequent smelting operations, which have caused unfavorable consequences to human health and aquatic environments. The State of Zacatecas (Mexico) is one of the most affected places by pollution from the mining industry. In this sense, the objective of this work is to present the results of radioactivity and heavy metal content in soil samples collected in mining areas of the State of Zacatecas, Mexico, as an example of artisanal and small-scale mining and its impact in the environment.

For this purpose, 21 samples from two areas have been collected (6 samples from Zone A and 15 samples from Zone B) to evaluate the level of radioactivity and the degree of contamination by heavy metals.

The activity concentration for ^{238}U and ^{232}Th is within typical values, but ^{226}Ra exceeds the value of 60 Bq kg- 1 in both areas. In some places, the concentration of ^{40}K is higher than the world average, according to UNSCEAR. The radium equivalent activity (Ra_{eq}) and absorbed Dose (D) indicate that some sites present a radiological risk for the population. Excess Lifetime Cancer Risk (ELCR) presents a higher risk than the world average in both sampled areas. Other parameters, such as the radiation index R_i, the external risk index H_{ex}, and the internal risk index H_{in}, also indicate that there is a greater risk due to radiation exposure in these areas.

In the case of heavy metals, some parameters, such as the Enrichment Factor (EF), the geoaccumulation index (I_{geo}), and the Contamination Factor (CF), show that some places in Zone A and Zone B are contaminated with arsenic and lead. In addition, the concentration of selenium obtained by ICP-MS in the sampled soil is higher than the average in the Earth's crust, both in mine waste dumps and in unaltered soil, which indicates that the background concentration for selenium in these places is higher than the world average.

Audience Take Away Notes

- The public will be able to learn how to evaluate the radioactivity and heavy metal levels in a mining area
- Additionally, it will be provided an interpretation of the results obtained
- Furthermore, this study supply information on the problem of abandoned mining areas, which should be reclaimed

Biography

Dr. M. Belen Gomez Mancebo studied Chemistry at the Complutense University, Madrid (Spain) and graduated in 1994. She then joined the research group of Prof. Carmen Camara at the department of Analytical Chemistry, at the Complutense University, Madrid (Spain). She received her PhD degree in 2002 at the same institution. After a three months postdoctoral fellowship supervised by Dr. R. Morabito at the National Agency for New Technology, Energy and The Environment (ENEA), Italy, she worked during three years in PPQF, Alcala de Henares University. Finally, she got a position as a senior scientist at CIEMAT, Madrid (Spain). She has published more than 40 research articles in SCI(E) journals.



M. R. Bissengaliyeva[1]*, M. A. Bespyatov[2], D. B. Gogol[1], D. T. Sadyrbekov[1]

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Method for correcting experimental values of the heat capacity of REE compounds by the debye temperature

This paper considers a method for correcting deviations in the heat capacity of the compounds of Rare Earth Elements (REE) having an anomalous contribution to the heat capacity and for which there is an isostructural compound without additional contributions. For example, erbium and thulium titanates are such compounds, the heat capacity of which was measured by adiabatic calorimetry. The splitting of the main term of paramagnetic Ln^{3+} ions with an incomplete 4f-shell by the crystal field removes the degeneracy of the Stark levels, the thermal population of which by electrons leads to the appearance of a Schottky contribution to the heat capacity. An isostructural analogue for them is lutetium titanate $Lu_2Ti_2O_7$, which is a diamagnetic compound.

Owing to the characteristics of the measurements, there is an increased scatter of experimental points from the smoothed curve over the temperature range from approximately 45 to 70 K. Nevertheless, it does not go beyond the 95% confidence interval. However, upon isolating an additional constituent of the heat capacity (Schottky contribution) composing a small value relatively to the total heat capacity, these deviations become noticeable and can affect the form of the anomalous component.

For a more accurate calculation of the lattice component of the heat capacity, a correction is used for the temperature dependence of the characteristic Debye temperature.

$\vartheta_D(Lu)/\ \vartheta_D(Ln) = [M_r(Ln)/M_r(Lu)]^{1/2}$.

After subtracting the lattice heat capacity, upon availability of deviations in the anomalous component, for correction the smooth sections of the dependence are described by suitable equations, to which the deviated values are reduced within the typical scatter of the experimental points in the given temperature range.

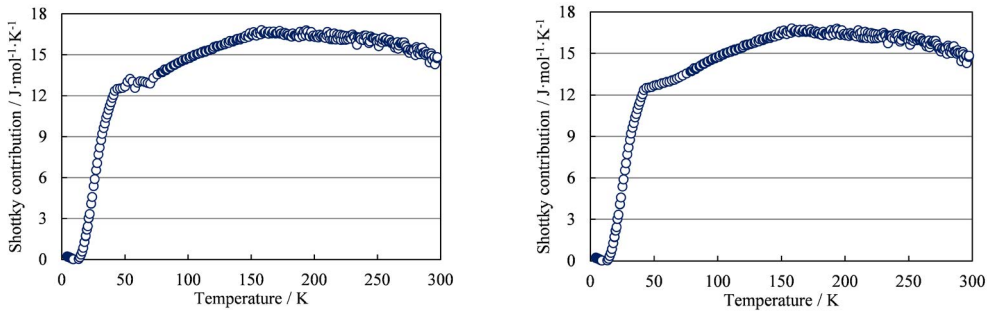


Figure - Schottky heat capacity for Tm_2Ti_2O7 before (left) and after (right) correction.

The corrected dependences are used to calculate the energy parameters of the Stark levels (level energy E_i and degeneracy factor g_i).

Audience Take Away Notes

- Obtaining novel data on the heat capacity, thermodynamic functions and magnetic properties of REE compounds
- Methods for isolating heat capacity components and physicochemical interpretation of the results from the standpoint of crystal field theory
- Identifying patterns in paramagnetic and ferromagnetic materials with cooperative and non-cooperative interactions
- Widening scientific knowledge on the properties of rare earth elements promotes the development of a technological and energy sector of industry, including green energy, wind power engineering, and hydrogen energy

Biography

Dr. Bissengaliyeva studied Chemistry at the Karaganda State University and graduated as MS in 1977. She then joined the research group of Prof. Bekturganov at the Abishev Chemical-Metallurgical Institute, Kazakhstan Academy of Sciences. She received her PhD degree in 1990 at the same institution. Since 2004 she has been working at the Institute for Institute of Problems of Complex Development of Mineral Resources as Head of the Mineral Processing Laboratory. In 2010 she received the academic degree of Doctor of Sciences (Chemistry) and the academic title of Full Professor. She has published more than 80 research articles in scientific journals.



Neila Bekturganova[1]*, Inna Kolesnikova[1], Aiganym Ismailova[1], Alexsander Suvorov[2], Ainur Tukhtamisheva[1]

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The use of polysiloxanes to improve the performance properties of cement

The development of methods for the directional formation of a durable structure of composite materials, obtaining products with specified performance properties with maximum simplicity of production technology and saving expensive raw materials is a priority task of any branch of the economy. In particular, in the construction materials industry. In the near future, concrete remains one of the main building materials. When considering concrete as a composite of coarse and fine aggregate, cement stone, water, and air pores, it is possible to formulate the main task of micro-, nanomodification as regulating the process of forming the structure of the material from the nanoscale to the macrostructure of the concrete mixture, as well as controlling the kinetics of the entire spectrum of chemical reactions accompanying the hardening process. Research on the properties of materials containing nanoparticles and nanostructures, the development of theoretical concepts of material modification, the development of specific technologies for obtaining new materials are priority areas of modern technologies and, in particular, technologies for the development of new building materials with specified properties. This task can be solved either by synthesizing new polymers or by modifying existing ones. The possibilities of synthesizing new polymers are limitless, but the technical and economic feasibility puts limits on its practical implementation, giving way to rich possibilities of physico-chemical and physical modification. Modern methods of prescription and technological modification of building materials have almost exhausted themselves. Building materials, including polymer materials, are composites with a clearly defined and developed phase boundary - this is the basis for successful improvement of properties by introducing various types of modifiers. The creation of polymer composites modified by the introduction of micro- and nanoparticles ensures a change in the structure of the matrix and leads to a significant improvement in operational characteristics.

In the present work, the physicochemical characteristics of the polysiloxane synthesized by us based on a reaction mixture of octomethylcyclotetrasiloxane, hexamethylsiloxane, sulfocationite resin intended for use as a micro- and nanomodifier in cement stones and concretes are investigated.

The mineralogical, chemical compositions and effective indicators of dispersion, density, rheological, and chemical activity of some raw materials – cement of various grades, crushed stone, sand, fly ash, etc. have also been determined.

Audience Take Away Notes

- Our research can be useful for researchers and materials scientists involved in improving the properties of concrete in the development of new or improved cements
- Of course, the results of our research can be used in conducting classes for students studying in the field of production of building materials
- These studies are carried out within the framework of a scientific project sponsored by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan and aimed at solving a specific task: improving the quality of cement mix

- We hope that it will improve the accuracy of a design, or provide new information to assist in a design problem

Biography

Bekturganova Neila-project manager, Candidate of Chemical Sciences, Professor. Participant of the international scientific project K-159 ISTC. Participant, responsible executor in more than 20 research projects of the Ministry of Science and Higher Education the Republic of Kazakhstan (1999-2017). The results of research work have been published in more than 100 scientific papers, including publications of 2 monographs. Her research interests include nano micromodifiers, structural and mechanical properties of dispersed systems of various nature, wastewater treatment.

Esraa Mohamed Musa[1,2], Faeza Alkorbi[1], Norah A. Alsaiari[1]*, Fatima A. Al Qadri[1,3], Raiedhah Alsaiari[1], Mabkhoot Alsaiari[1], Iman Mohammad.Shedaiwa[1,3], Mervate Mohamed Mohamed[1,4]

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[3]Department of Chemistry of Science faculty, Sana'a University, Yemen
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Phytochemical screening and anti-microbial activity of methanolic and aqueous extract of pink cabbages and red grape

In this study, the phytochemical composition, antioxidant potential, and antimicrobial effects against Grampositive bacteria, Gram-negative bacteria, and fungi in both aqueous and methanolic extracts of Brassica oleracea var. capitata (Pink Cabbages) and Red Grapes fruit belonging to the families: Brassicaceae and Vitaceae were determined. Methanolic extract of red Grapes exhibited high activity a giants Bacillus Subtilis and Staphylococus aureus. Additionally, it showed moderate and weak activity against Escherichia coli and fungi. Whereas methanolic extract of pink Cabbage exhibited high activity a giants Staphylococus aureus, moderate activity against Bacillus Subtilis. No activity was observed against Escherichia coli and fungi. Both aqueous and methanolic extract of red Grapes and Pink Cabbages are rich in alkaloids flavonoids, Tannins and Steroids.

However, Saponins, coumarins and Terpenoids are absent. The approximate analysis of both Red Grape and Pink Cabbages demonstrated: The study assessed the moisture content, ether extract, crude protein, crude fiber, ash, and non-free extract in pink cabbages. It observed that the antioxidant activity of the methanolic extract from pink cabbages, determined through DPPH radical scavenging activity, surpassed that of the methanolic extract from red grapes. In contrast, antioxidant activity of methanolic extract red Grape when ferrous iron-chelating was used to determine their antioxidants activity.

Biography

Norah Alsaiari is currently working as an Assistant professor at Najran university Saudi Arabia, Specialising in Organic Chemistry , In 2023 she completed her Ph.D. in Organic Chemistry at University of East Anglia, Norwich, UK, in the field of Porphyrins and phthalocyanines are heterocyclic macrocycle compounds that used as a building block to form multidecker complexes. She also completed her MSc in Organic Chemistry at Taif University ,Saudi Arabia. She Started as Teaching assistant at Najran university in 2009, she was then promoted as lecturer in 2012, and in December 2023 she became an Assistant professor .



L. P. Yunnikova, O. V. Pshenitsyna*
Perm State Agro-Technological University named after Academician D.N. Pryanishnikov, Perm, Russia

Nucleophilic functionalization of tropyl salts by heterocyclic amines, amides or hydrazides of carboxylic acids

The review provides information on new reactions of nucleophilic functionalization of tropylium salts with heterocyclic amines, amides or hydrazides of carboxylic acids.

The possibility of interaction of 2-aminopyridine with tropylium salts by replacing the hydrogen in the amino group of 2-aminopyridine with a tropylium fragment has been established. It has been established that the tropylium fragment can be displaced from N-(1'-cyclohepta-2', 4', 6'-trienyl)-2-aminopyridine by the more electrophilic tritylium cation. The isomers (3- and 4-aminopyridines and 4-aminoquinoline) behave identically towards the tropylium cation; as a result of the reaction, the corresponding N-tropylated products are obtained.

The interaction of tropylium salts with the pharmacophore 2-aminopyridine, 2-aminopyrimidine and 4,6-disubstituted pyrimidines occurs selectively at the exocyclic nitrogen atom of the amino group as a monosubstitution. However, the interaction of tropylium tetrafluoroborate with 2,6-diaminopyridine proceeds as a replacement of hydrogen at C3 and C5 of the cycle with the formation of 3,5-di(cyclohepta-2,4,6-trien-1-yl) pyridin-2,6-diamine, in which two amino groups remain free. The interaction of tropylium tetrafluoroborate with 2,5-diamino-1,3,4-thiadiazole or 3,5-diamino-1,2,4-thiadiazole proceeds as a disubstitution at two amino groups. The interaction of tropylium tetrafluoroborate with urea, thiocarbamide and sulfanilamide proceeds similarly.

In addition, non-benzenoid aromatic cations, when interacting with imidazole and benzimidazole, replace the hydrogen of the secondary amino group of the heterocycle with xanthilium, thioxanthilium or tropylium fragments.

By reacting low-basic aromatic amines with tropylium salts in the presence of imidazole, N-tropylation products with antimicrobial activity were obtained.

Audience Take Away Notes

- Interest in the chemistry of Non-Benzenoid Aromatic Cations (NACs) is largely associated with the search for substances with biological activity among their derivatives
- Tropylium salts are used in organic synthesis as catalysts, promoters or reagents. As Lewis acids (catalysts), they have found application in the acetalization reaction of aromatic aldehydes, and the functionalization of cycloolefins with aromatic aldehydes. In the oxidative functionalization of N-substituted tetrahydroisoquinolines, tropylium tetrafluoroborate is used as a promoter, which converts them into iminium intermediates for subsequent reaction with nucleophiles
- The scientific and preparative value of accessible and reactive tropylium salts lies in the ease of their C- or N-functionalization with aromatic or heterocyclic amines, as well as amides or hydrazides of monocarboxylic acids. Tropylium salts are used as effective reagents in the synthesis of 4-(7-cyclohepta-1,3,5-trienyl)-aniline and 4-(7-cyclohepta-1,3,5-trienyl)-N-cyclohepta-2,4,6-trienyl)aniline, which have pronounced antimicrobial activity

- This review summarizes information on non-catalytic reactions of tropylium salts with heterocyclic amines of the series 2-aminothiazole, 5-aminotetrazole, aminopyridines, aminopyrimidines, as well as with amides of sulfanilic, thio- and carbonic acids; diamines of the pyridine series or thiadiazoles

Biography

Olga Pshenitsyna from Federal State Budgetary Educational Institution of Higher Education Perm State Agricultural and Technological University named after. D.N. Pryanishnikova.



U. V. Mammadova[1], I. T. Nageva[2], L. M. Gasanova[1], T. M. Nagiev[1,2]*

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Oxidative transformation of ethylene into ethyl alcohol and acetaldehyde under the per-FTPhPFe^{3+}OH/Al_2O_3 bioimitator

For the first time, the investigation of the coherent-synchronized reaction of heterogeneous catalytic ethylene monooxidation with hydrogen peroxide into ethyl alcohol and acetaldehyde was carried out using the new highly efficient bioimitator, per-FTPhPFe^{3+}OH/Al_2O_3, which is highly resistant to oxidizing agents and high temperatures, as well as a long service life. The process of gas-phase ethylene monooxidation with hydrogen peroxide was carried out at atmospheric pressure, in a flow system, in an integral type reactor with a reaction zone volume of 3.5 cm^3. Optimal conditions for maximum yields of target products were determined: a) at a temperature of 120°C, a concentration of an aqueous solution of hydrogen peroxide of 20 wt.%, molar ratio C_2H_4:H_2O_2 = 1:1, the highest yield of ethyl alcohol is 15.4 wt.%. The selectivity for monooxygenase products is almost 100%; b) at t = 200°C, concentration of an aqueous solution of hydrogen peroxide 30 wt.%, molar ratio C_2H_4:H_2O_2 = 1:1.7, the yield of acetaldehyde is 34.6 wt.%. The selectivity for monooxygenase products is 87%.

The process of biomimetic oxidation of ethylene by hydrogen peroxide is carried out in the bioimitator-H_2O_2-C_2H_4 system in a bifurcation mode, in which catalase (decomposition of hydrogen peroxide), monooxygenase (ethylene monooxidation) and peroxidase (peroxidase oxidation of ethyl alcohol) reactions are coherently proceed. The oxidative conversion of ethylene into monooxygenase products occurs in the following sequence: $C_2H_4 \xrightarrow{ImtOH,H_2O_2} C_2H_5OH \xrightarrow{ImtOH,H_2O_2} CH_3CHO$. Each of these transformations is a complex reaction and consists of two coherent-synchronized reactions: 1) primary (catalase) and 2) secondary (monooxygenase and peroxidase) reactions. The mechanisms of ethylene oxidation into ethyl alcohol and acetaldehyde on the surface of a biomimetic catalyst are presented, in which the unity of redox and acid-base mechanisms can be traced within the framework of the bond Redistribution Chain (BRC) theory.

Kinetic modeling of the process of heterogeneous catalytic ethylene monooxidation with hydrogen peroxide on the per-FTPhPFe^{3+}OH/Al_2O_3 bioimitator was carried out using various methods: using the Michaelis-Menten equation; using the method of stationary concentrations; based on the determinant equation. A comparative analysis of the results obtained by various modeling methods showed that the kinetic model using the determinant equation adequately describes the processes. It has been established that the kinetic model, based on the determinant equation and the coherence relationship of coherent-synchronized catalase, monooxygenase and peroxidase reactions allows assessing the coherent nature of synchronously flowing reactions qualitatively and quantitatively. Kinetic modeling was also carried out with the aim of further application of the chosen model in the optimization and design of this process.

Biography

Tofik Nagiev is a Vice-president of Azerbaijan National Academy of Sciences, Director of Research Center of Azerbaijan National Encyclopedia and Department chief of Nagiev Institute of Catalysis and inorganic chemistry of ANAS. The Professor of the department of the physical and colloid chemistry of Baku State University. He is author of the monography Coherent Synchronized Oxidation Reactions by Hydrogen Peroxide, Amsterdam: Elsevier, p. 325, 2007.



Vladimir Voronov
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Use of high-resolution NMR spectra transformed by paramagnetic complexes for studying molecular structure

This paper provides an overview of the features specific to the Nuclear Magnetic Resonance (NMR) of paramagnetic molecules. These features can be attributed to the hyperfine or electronic coupling between unpaired electrons, which are localised on the coordinating ion, and слов) resonant nuclei. That leads both to the paramagnetic broadening and to the paramagnetic shifts (contact and pseudo-contact ones) of resonance lines in the NMR spectra. A contact shift is observed when the probability of an unpaired electron location in the place of a resonant nucleus differs from zero. Therefore, these shifts constitute a source of information on the nature of the metal-ligand bond as well as on the ligand electronic structure. Pseudo-contact shifts characterise the spatial structure of the molecule, thus being important for solving various structural problems. Thus, the study of the NMR phenomenon in paramagnetic systems makes it possible to obtain important information about the structure of multielectron systems. Paramagnetic shifts are much larger than chemical shifts in the spectra of diamagnetic compounds and, in addition, have a characteristic temperature dependence. For paramagnetic substances, various relaxation effects are possible, which significantly expands the possibilities of NMR as a research method. In particular, the study of temperature dependence Paramagnetic shifts and amplification of signals make it possible to find the thermodynamic parameters of the process of complexation in solution, to study the stoichiometry of complexes, as well as the mechanisms of league exchange. This paper covers pioneering works describing the specifics of the NMR spectra transformed by adding paramagnetic complexes of iron-group elements on the example of cobalt and nickel complexes, as well as complexes of rare-earth elements on the example of europium (Hinckley C.C., Sanders J.K.M. and Williams D.H., Molin Yu.N. and Zaev E.E. with colleagues). We present main features of the paramagnetic additive's method, allowing resolution of difficulties associated with large paramagnetic broadening of resonance lines in high-resolution NMR spectra. Of iron-group elements, a paramagnetic ion Co^{2+} is shown to be an effective shift reagent. In some cases, a Ni^{2+} ion may also be used for this purpose.

Biography

Professor Vladimir Voronov's research interests are related to solving problems of molecular spectroscopy and physico-organic chemistry by methods of nuclear magnetic resonance and quantum chemistry. In addition, for the last twenty years or so, his research interests have included scientific and methodological issues related to cognitive barriers of university students. He is the author of more than three hundred publications in periodicals, including more than thirty books. He received a number of awards established by the Russian Academy of Natural Sciences, including the Gold Medal For innovative work in the field of higher education. Member of the American Chemical Society.



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Aniline quinones produce mitochondrial dysfunction and migrastatic effect on triple-negative breast cancer line MDA-MB-231

Triple-Negative Breast Cancer (TNBC), a subgroup that does not express estrogen, progesterone, and HER-2 receptors, is responsible for 20% of new cases. TNBC is characterized by a poor prognosis and absence of specific therapies, associated with a four-fold increased risk of metastasis. Current treatments act on the uncontrolled cancer cell proliferation of cancer cells but do not inhibit their migration and invasion. This represents an urgent need to obtain new drugs that selectively the metastatic cascade. Tumor cells have diverse metabolic phenotypes, exhibiting variable contributions of glycolysis and oxidative phosphorylation. In them, the mitochondrial electron transport chain has been identified as an essential component of bioenergetics, biosynthesis, and the redox control of cancer proliferation and metastasis, being a promising pharmacological target in metastasis. Many natural and synthetic naphthoquinones, such as juglone, plumbagin (a derivative of vitamin K_3), 1,4-naphthoquinone, and menadione, have been studied for possessing pharmacological activities by interacting with traditionally validated therapeutic targets, such as altering kinase activity and activating or deactivating signaling pathways. Also, redox compounds increase the cellular oxidative stress, an important mechanism of their cytotoxicity. Plumbagin, with an effect on several types of cancer, including breast cancer, has been reported as a potent antitumor capable of inhibiting the process of Epithelial-Mesenchymal Transition (EMT) that confers resistance to therapy endocrine against cancer.

In this study, we evaluated a series of amino quinone derivatives as potential antitumor compounds that affect the mitochondrial metabolism through the inhibition of complex I in TNBC, which reduces cell migration in vitro. The structure-activity relationship of amino quinone derivatives was evaluated. The results revealed that the RL-4 derivative selectively affected cell viability in cancer cells (1, 5, and 10 μM) and decreased their clonogenic capacity, which was reversed for pyruvate addition. It generated a decrease in OCR and an increase in ECAR. This shows a metabolic change towards glycolysis due to a possible inhibition of complex I. With the consequent increase in ROS, decrease in mitochondrial membrane potential, and inhibition of cell migration (5 and 10 μM) in addition to reversing the migration promoted by doxorubicin, a drug used as chemotherapy.

Audience Take Away Notes

- The audience will be able to learn the basic structure of some naphthoquinone molecules that, due to their structure, can act as potential mitochondrial targets and intervene mainly in the mitochondrial function of tumor cells due to their impaired mitochondrial function
- This research proposes the use of a potential target for cancer treatment aimed at preventing metastasis, such as mitochondria. Since current cancer treatments are directed at cell proliferation, this research opens a range of possibilities in the study of synthetic molecules based on scaffolds of molecules that occur in nature to avoid the formation of new tumor foci, which in most cases leads to the death of the tumor patient

- Other benefits are
    - Decreased cytotoxicity of conventional cancer treatments
    - Better prognosis and quality of life for patients with triple-negative breast cancer since they would avoid the terrible side effects caused by chemotherapy, their only treatment
    - It is an innovative approach that aims to avoid metastasis, which would decrease the mortality rate
    - It contributes to the knowledge of basic science since the mechanism of action can be studied, and the effects of molecules can be improved simply with minor changes in their structure

Biography

Doctoral student Yarcely Rodríguez studied biology at the Central University of Venezuela, developing her thesis in the molecular genetics laboratory of Dr. Takiff at the Venezuelan Institute of Scientific Research, graduating in 2011. She then joined the laboratory for the synthesis of bioactive compounds led by Professor Araya Maturana at the Institute of Chemistry of Natural Resources of the University of Talca-Chile and Interdisciplinary Group on Mitochondrial Targeting and Bioenergetics (MIBI), where she is finishing her doctoral thesis work to receive the title of doctor.



Ying Huang Lai
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Nickel single atoms enhance graphitic carbon nitride for superior photo-electrocatalytic hydrogen evolution

In this study, we propose to use g-C_3N_4 as a carrier to chemically mobilize metal atom nickel on g-C_3N_4 . The composites were then used to prepare electrodes, and the photoelectric catalyst was activated by applying a constant potential (−0.10 V vs. RHE, no IR compensation). Through detailed property analysis by X-ray Absorption Spectroscopy (XAS), X-ray Photoelectron Spectroscopy (XPS), Photoluminescence (PL), Thermogravimetric Analysis (TGA) and Cyclic Voltammetry (CV), we showed that the Ni modified on g-C_3N_4 is single-atom-loaded onto g-C_3N_4 to form the active center of the photoelectric catalyst. The catalysts were tested by HER activity. The best-performing catalyst has a Ni load of 23 μg/cm^2 on the electrode, with a weight percentage of 2.6%. Under acidic conditions, at η = 50 mV, the turnover frequency for photoelectric catalysis is ~17.3 H_2/s. The reaction mechanism of this series of catalysts for HER exhibits a Tafel slope of ca. 50 mV/dec in the low-potential region, and the Heyrovsky reaction is the rate-determining step. The photoelectric catalyst (Ni/g-C_3N_4) exhibits high stability during long-term HER process. The decline rate after 1000 cycles of HER is less than 5%. Compared with Pt atoms supported on carbon materials, the cost of Ni/g-C_3N_4 catalysts shows strong competitiveness in the HER process.

Audience Take Away Notes

- The audience can gain insights into the feasibility of using sparse atomic catalysts for catalytic reactions
- Understanding evaluation methods for hydrogenation reactions
- Catalyst design concepts applicable to other heterogeneous catalysts

Biography

Dr. Ying Huang Lai pursued his studies in Chemistry at the Department of Chemistry, National Tsing Hua University, Taiwan, in 1997, and obtained his Master's degree in 1999. He continued his doctoral studies within the same department and acquired his Ph.D. in 2003. Following a four-year postdoctoral research supervised by Dr. U-Ser Jeng at the National Synchrotron Radiation Research Center, he secured a position as an Assistant Professor of Chemistry at Tunghai University. He has published over 50 research articles in SCI journals.



López-Cabaña Zoraya[1], Pariguana- Begazo Manuel[2], Parra-Sepúlveda Cristian[3], González-Gutiérrez Liz[3], García-Cancino Apolinaria[3], Alderete-Triviños Joel[1]

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Selenium nanoparticles stabilized in tannic acid: An innovative approach for combating infections caused by H. Pylori or Candida albicans

Selenium is an essential trace elemental in the diet, required for maintenance of health and growth. Give that the least toxic form of selenium is elemental Se, its nano-form has attracted significant attention. In recent years, selenium nanoparticles (SeNps) attracted the interest of many researchers due to their biocompatibility, bioavailability and low toxicity. Several studies have pointed out the ability of SeNps to exhibit anticancer, antioxidant, antibacterial and anti-biofilm properties. So far, remarkable antimicrobial activity of these nanoparticles have been evidenced against pathogenic bacteria, fungi and yeasts. The recent boom in nanotechnology furnished and indefinite number de applications of metal nanoparticles in biomedicine. Metal nanoparticles, for example, gold and silver, have immense medicinal benefits but are costlier to synthesis, whereas the synthesis of SeNps is economical and they can be integrated with other biological agents to enhance their biological properties. The synthesis of SeNps by various methods has been reported. These methods are divided two categories, namely biological and chemical reduction. The chemical reduction method uses chemical reducing agents, energy sources and apparatus to carry out the reaction. So far, SeNps have been synthesized in various forms such as nanowires, nanorods and nanotubes through sonochemical, microwave, hydrothermal methods. In this study, we discuss the synthesis of SeNps using tannic acid as reducing and stabilizing agent, and explores their potential as a novel strategy against bacterial (H. pylori) and fungal (Candida albicans) infections. Tannic acid, a plant derived polyphenolic compound, is one such agent which embodies characteristics of being harmless and environmentally friendly combined with being a good reducing and stabilizing agent, these gives an eco-friendly agent to the green synthesis of SeNps. The synthesis of monodisperse SeNps by tannic acid was conducted under slightly basic conditions (pH=8). The characteristic absorption peak of the SeNps appearance of a sharp peak at 265 nm. The DRX pattern show the reflections corresponding to metallic Se. In humans, fungal and bacterial infections are responsible for causing a wide range of diseases to life-threatening. Infections caused by Helicobacter pylori (H. pylori), a Gram-negative microaerobic bacterium that colonizes the human stomach, it has been associated with gastrointestinal diseases including chronic gastritis, peptic ulcer, gastric carcinoma. On the other hand, Candida albicans is the most common pathogenic fungus that affects the oral cavity, skin, reproductive tract, and gastrointestinal tract. These microbial infections that cause great health concerns are due that most of the pathogenic organisms have become drug-resistant because of the constant utilization of a wide range of antibiotics. The frequency percent of Minimun Bactericidal Concentration (MIC) (µg/mL) of SeNps in clarithromycinsensitive and resistant H. Pylori isolates was determined. SeNPs showed antibacterial activity against both clarithromycin sensitive and resistant H. Pylori isolates with MIC values of 2.9 - 370 µg/mL. The dispersion of the MIC of SeNPs in clarithromycin sensitive isolates was 37.5 ug/ml and in clarithromycin resistant isolates was 37.5 to 92.5 ug/mL. This results demonstrate the potential of SeNps as novel antimicrobial agents for the treatment of diseases caused by H. pylori and candida albicans.

Audience Take Away Notes

- Our study involves transdisciplinary research focused on the use of nanotechnological tools for the design of novel materials with applications in medicine.
- The appropriate clinical use of novel antimicrobial agents based on metallic nanoparticles could prevent the emergence of microbial resistance.

Biography

Dr. Zoraya López Cabaña studied Chemistry at the Carabobo University, Venezuela and graduated in 2000. She studied Magister Scienciarum in Chemistry at the Venezuelan Institute of Scientific Research, Venezuela (2004) supervised by Prof. Gema González. She then joined the research group of Prof. Guillermo González and she received her PhD degree in 2009 at the Chile University, Chile. After one-year postdoctoral fellowship supervised by Prof. Leonardo Santos at the Chemistry Institute of Natural Resources (IQRN), Talca University, Chile, she obtained the position of Conferenciante Professor at the IQRN. She has published more than 25 research articles in SCI(E) journals.

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