5TH EDITION OF

CHEMISTRY WORLD CONFERENCE

JUNE 02-04, 2025

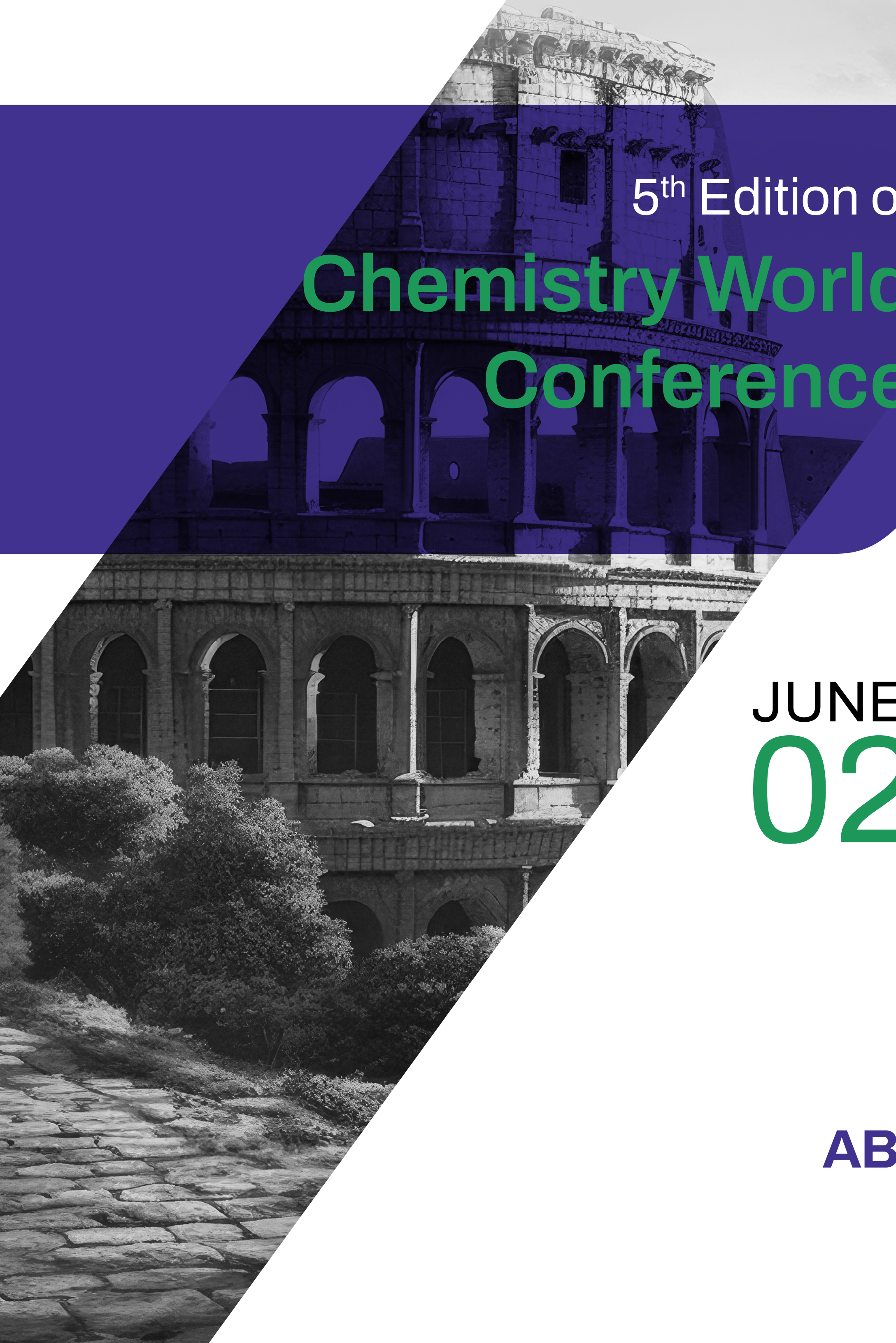
ROME, ITALY

VENUE

NH VILLA CARPEGNA VIA PIO IV, 6, 00165 ROMA RM, ITALY

BOOK OF ABSTRACTS

magnus Group



5th Edition of

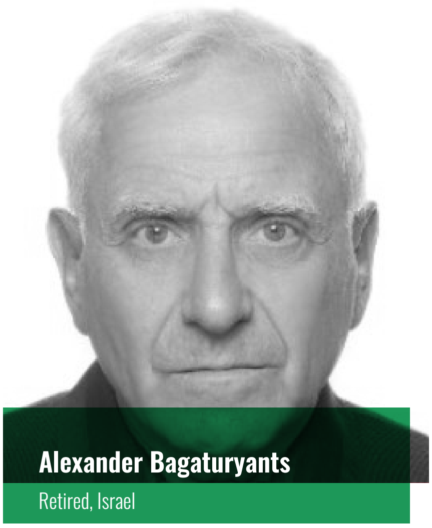
Chemistry World Conference

JUNE
02-04
2025

BOOK OF
ABSTRACTS

Index

Keynote Speakers

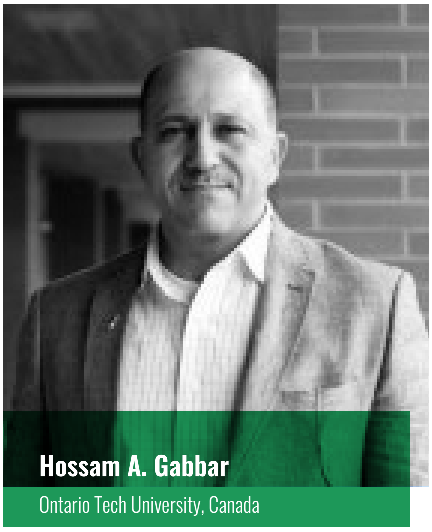


Alexander Bagaturyants

Retired, Israel

Haibo Ge

Texas Tech University, USA



Hossam A. Gabbar

Ontario Tech University, Canada

Kyeongjae (KJ) Cho

UT Dallas and BEACONS, USA

Serge Cosnier

Silesian University of Technology, Poland

Sergey Suchkov

National Center for Human Photosynthesis,
Aguascalientes, México

Shree Niwas Chaturvedi

Centre for Aptitude Analysis and Talent Search, India

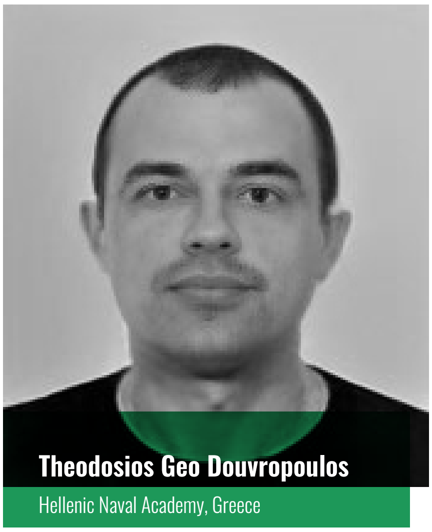
Silvia Elizabeth Asís

Universidad de Buenos Aires, Argentina

Stanislaw Dzwigaj

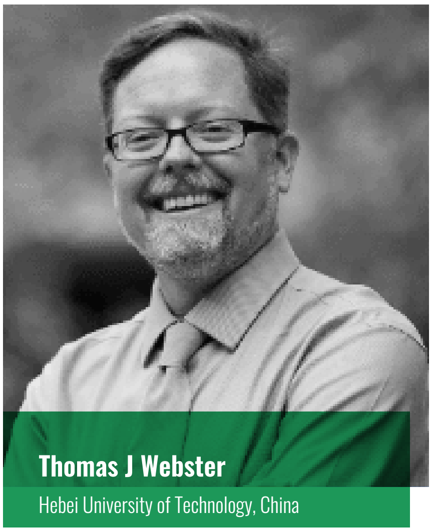
Sorbonne Université, France

Keynote Speakers



Theodosios Geo Douvropoulos

Hellenic Naval Academy, Greece



Thomas J Webster

Hebei University of Technology, China

Yong-Xiao Wang

Albany Medical College, USA

Thank You
All...

Welcome Message

Welcome to Chemistry World Conference 2025, an extraordinary gathering of the brightest minds in chemistry from across the globe. This conference brings together leading researchers, scientists, and industry professionals to explore the latest breakthroughs and transformative advancements shaping the future of chemistry.

Chemistry 2025 promises an engaging and dynamic program with a wide range of scientific sessions that are sure to spark innovative research presentations. Together, we will explore the full spectrum of chemistry, spanning organic and inorganic chemistry, biochemistry, physical chemistry, and cutting-edge interdisciplinary studies in medicine, industry, and food, providing invaluable insights and fostering impactful collaborations.

This conference is designed to inspire and energize our collective mission to revolutionize chemistry and unveil solutions to some of the world's most pressing challenges. It is an exceptional opportunity to exchange ideas, share knowledge, and envision a more sustainable and innovative future. See you soon!

Prof. Dr. Serge Cosnier

Gliwice-Grenoble, Poland-France

Welcome Message

Dear Colleagues, Scientists, Bioengineers and Friends,

On behalf of the Organizing Committee, it is my pleasure to invite YOU from all over the world to Welcome to the 5th Edition of Chemistry World Conference" (Chemistry 2025), set to unfold in the historic city of Rome, Italy, from June 02-04, 2025.

This Event is contributing to the further improvement of global chemistry in its very broad scope of fields, trends and applications, including canonical organic, physical and inorganic chemistry, analytical chemistry, medicinal chemistry, biochemistry and associated drug discovery, polymer chemistry, surface chemistry and even quantum chemistry describing the motion and interaction of subatomic particles in atoms and molecules. This highlights the multi- and inter-disciplinary nature and very broad scope of catalysis and chemical engineering and will provide all participants a catalytic opportunity to exchange ideas, learn from each other and initiate collaborations.

One of the key features of the Conference is to exchange breakthrough ideas in the field of biocatalysis and chemical engineering to promote top level research by focusing on the recent trends. In this context, design and synthesis of new materials would be one of the most important part of global chemistry. Those perspective aspects will provide us with new angles to look at the chemistry in the coming decades and inspire the development of new methods, technologies and strategies to illustrate the Chemistry as a core element of a Changing World.

Keynote speeches will be given by distinguished scholars and experts from academic institutions and industry, and oral presentation by delegates and poster presentations by young junior participants.

This conference will provide excellent opportunity to establish highly productive relations and collaborations for future research and projects. So, your participation and contributions are fundamental to the success of this Conference. Together, we aspire not only to deepen our collective understanding but also to propel innovation within catalysis and design-driven chemical engineering.

WE hope to see you all in Grand Rome, to enjoy the event along with the exceptional beauty of the ancient and unique historical City. We extend a heartfelt welcome on this occasion and will have an appealing, exciting and unforgettable experience and thank you!

Dr. Sergey Suchkov, MD, PhD

N.D. Zelinskii Institute for Organic Chemistry of the Russian Academy of Sciences,
Moscow, Russia

Centro de Estudios de la Fotosíntesis Humana, Aguascalientes, México

Welcome Message

Dear Conference participants, it is an honor and pleasure for me to write a few welcome notes. Chemistry today makes unprecedented progress, because it not only penetrates into all the areas of human activities, but also determines progress in very important directions. Chemistry plays a fundamental role in providing global sustainable development. All these aspects are reflected in the topics of this Conference, which encompass almost all conceivable areas of human activities, from analytical and medicinal chemistry to industrial chemistry. I wish all of the Conference participants great success in their presentations and in obtaining new knowledge and skills in adjacent areas of scientific exploration.

Prof. Dr. Alexander Bagaturyants

Retired, Israel

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 2025

The **5th Edition of the Chemistry World Conference** is a premier global event set to take place in **Rome, Italy**, from **June 02–04, 2025**. This esteemed gathering will bring together leading scientists, researchers, chemists, chemical engineers, and industry professionals from around the world to exchange knowledge and explore the latest advancements in the field of chemistry.

Themed “**Chemistry: Innovations, Applications, and Sustainability,**” the conference highlights the pivotal role of chemistry in addressing global challenges and driving progress in materials science, engineering, biology, and environmental science.

Participants can look forward to a dynamic and comprehensive agenda, including keynote lectures, interactive workshops, oral and poster presentations, and valuable networking opportunities. Esteemed speakers from academia, industry, and research institutions will share insights into cutting-edge research, emerging trends, and transformative technologies in chemistry.

The Chemistry World Conference 2025 offers a unique platform for intellectual exchange, professional development, and global collaboration, uniting like-minded individuals dedicated to shaping a sustainable and innovative future through chemistry and its allied fields.

Table of Contents

Table of Contents

Table of Contents

Table of Contents

Table of Contents

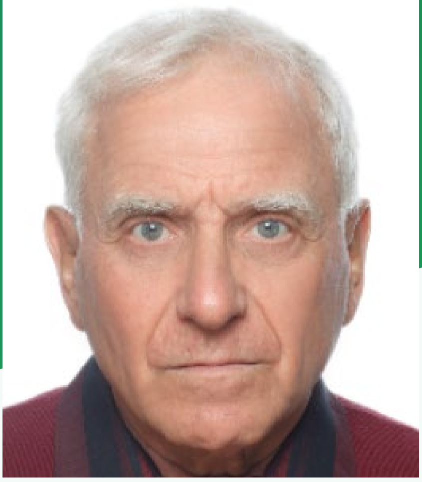
5th Edition of

Chemistry World Conference

JUNE
02-04
2025

KEYNOTE PRESENTATIONS

Biography



Prof. Alexander Bagaturyants is now retired. He has been full professor at National Research Nuclear University "MEPhI" and chief researcher at Photochemistry Center of the Russian Academy of Sciences. He was graduated from D.I. Mendeleev Institute of Chemical Technology, Moscow, Russia in 1962, obtained his PhD degree, Dr. Sci. degree, and the academic title of Professor in 1968, 1987, and 1992, respectively, all in physical chemistry. His main research interests are in the field of atomistic multiscale simulations of organic functional materials and in the application of theoretical methods in organic nanophotonics. He is the author of 105 articles in SCI(E) journals.)

Alexander Bagaturyants

National Research Nuclear University "MEPhI", Israel

Theoretical Modeling in organic nanophotonics: Processes and devices

Multiscale atomistic simulation methods are applied to studying excited molecules in organic materials and their interaction with neighboring molecules. The formation of exciplexes at the interface between layers of organic molecules in multilayer structures, typical for organic light-emitting diodes and for other devices of organic electronics and photonics, makes an important contribution to their emission spectrum. Adequate models of a complex system containing excited components and suitable methods for the description of charge and/or excitation transfer are considered. These following steps are briefly discussed: (1) the construction and use of the library of parameters of the EFP (Effective Fragment Potentials) approximation for the simulation of environment of luminescent dopants and transport molecules in the layers; (2) the estimation of the accuracy of the obtained results; (3) the creation of a program complex for the construction of the polarized environment using the library of parameters in the EFP approximation; (4) the investigation of the effect of the polarized environment on the positions of triplet and singlet levels of luminescent dopants; (5) the development and improvement of approaches to the calculation and interpretation of absorption spectra of supramolecular systems using hybrid QM/MM methods; (6) a molecular dynamics study of the formation of exciplexes at the interface between two organic semiconducting layers and calculations of their properties by quantum chemical methods; (7) development of force fields for metal-organic complexes for molecular dynamics simulation of such systems; (8) the use of multiconfigurational quantum-chemical calculations of radiative and intersystem crossing constants; (9) studying spin-mixed states of phosphorescent iridium(III) complexes, (10) the mechanism of charge separation in bulk heterojunction organic photovoltaics; (11) application of theoretical methods to molecular organic light-emitting and photovoltaic devices.

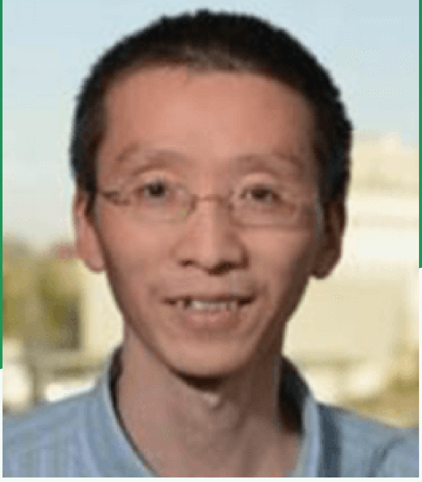
Haibo Ge

Department of Chemistry & Biochemistry, Texas Tech University, Lubbock, TX, USA

Distal functionalization via transition metal catalysis

The ubiquitous presence of sp3 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 sp3 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, sp3 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.

Biography



Haibo Ge received 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, began independent academic career at the Indiana University–Purdue University Indianapolis and relocated to Texas Tech University in 2020. Research by 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.

Biography

Hossam A. Gabbar Professor, P. Eng., Fellow IET (FIET), 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

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.

Dr. Gabbar is a full Professor in the Faculty of Energy Systems and Nuclear Science, and cross appointed in the Faculty of Engineering and Applied Science, at Ontario Tech University (UOIT), has established the Energy Safety and Control Lab (ESCL), Smart Energy Systems Lab, and Advanced Plasma Engineering Lab. Dr. Gabbar is the recipient of the Senior Research Excellence Aware for 2016, UOIT. Recognized among the top 2% of worldwide scientists with high citation in the area of energy. He is a Distinguished Lecturer of IEEE NPSS, and is a Fellow IET (FIET). Dr. Gabbar is leading national and international research in the areas of smart energy grids, energy safety and control systems, and waste-to-energy using advanced plasma technologies. Obtained B.Sc. degree in 1988 with first class of honor from the Faculty of Engineering, Alexandria University (Egypt). In 2001, obtained Ph.D. degree from Okayama University (Japan). From 2001 till 2004, joined Tokyo Institute of Technology (Japan), as a research associate. From 2004 till 2008, joined Okayama University (Japan) as an Associate Professor, in the Division of Industrial Innovation Sciences. From 2007 till 2008, Dr. Gabbar was a Visiting Professor at the University of Toronto. He also worked as process control, safety, and automation specialist in energy and oil & gas industries. Has more than 290 publications, including patents, books / chapters, journal, and conference papers.

Biography

Dr. Kyeongjae (KJ) Cho is a full professor and BEACONS Center director at UT Dallas and received PhD (1994) in Physics from MIT, worked as a postdoctoral associate (1994-1995), research scientist (1995-1997) at MIT (a jointly at Harvard University during 1995-1996), assistant professor at Stanford University (1997-2006), and a faculty member at UT Dallas since 2006. Dr. Kyeongjae received Frederich E. Terman Award (1997), was elected as a Fellow of the Institute of Physics (2004) and a fellow of the American Physical Society (2016). Has been published more than 440 journal articles (Google Scholar: h-index=96, total citation=45,527).

Kyeongjae (KJ) Cho

Department of Materials Science and Engineering and BEACONS Center, University of Texas at Dallas, Richardson, TX, USA

Rational design of battery cathode materials

Current Li Ion Batteries (LIBs) are improved versions of the 1991 Sony LIB based on graphite anode, organic liquid electrolytes, and $LiCoO_2$ layered oxide cathode. In the commercial applications of LIBs, cathode materials are known to be the critical component in determining the battery cost (~50% of material cost) and the energy storage capacity (cell capacity=~1/3 cathode capacity). Over the last 30 years, the initial $LiCoO_2$ cathode (~140 mAh/g charge capacity) has evolved to high capacity cathodes with increasing Ni content replacing Co starting from Li(Ni1/3Co1/3Mn1/3)O2 or NCM111 (~160 mAh/g) to NCM433, NCM532, NCM622, NCM721, NCM811 (~200 mAh/g), and LiNiO2 (>200 mAh/g). With 70-80% Ni in NCM cathodes (theoretical capacity of ~275 mAh/g), more than 70% of Li can be utilized in the electrochemical reactions in realizing the high-capacity cathode. However, in the fully charged state of LIBs, cathode materials are very unstable toward chemical reactions (irreversible reactions with electrolytes, oxygen evolution and phase changes) and mechanical degradation (interface crack formation). Specifically, the high-Ni NCM cathode materials are known to have large volume change (-7%) at 80% delithiation with the majority of volume change ($\Delta V/V=-5\%$) happening at Li delithiation from 70% to 80% leading to the mechanical cracking of the secondary cathode particles. In this talk, we will discuss multiscale modeling study based on density functional theory (DFT) calculations to examine the atomic and electronic structure origins of the cathode degradation mechanisms.

Serge Cosnier

Silesian University of Technology, Centre for Organic and Nanohybrid Electronics, Gliwice, Poland

CNRS Université Grenoble Alpes, Département de Chimie Moléculaire, Grenoble, France

Nanostructured biodevices based on carbon nanotubes and glyconanoparticles for bioelectrocatalytic applications

For four decades, the functionalization of electrodes by biomaterials based on electrogenerated polymers, carbon nanotubes and/or nano-objects, was widely used in the field of analytical chemistry and energy conversion for the design of biosensors and biofuel cells. Some new approaches for developing nanostructured biomaterials based on functionalized carbon nanotubes, will be briefly described as the compressions of carbon nanotubes, the self-assembly of carbon nanotubes in the form of buckypapers or the creation of hollow electrodes.

These different electrochemical materials combined with enzymes as catalytic element, will be applied to the design of glucose/oxygen enzymatic fuel cells and their performances will be compared. Examples of implantation of these biofuel cells in animals will be presented.

In particular, the concept of hollow bioelectrodes based on the assembly of two buckypapers was developed to generate a microcavity defined by the thickness of the glue linking the two sheets. These buckypapers are permeable only to water and enzyme substrates but not allow the permeation of enzymes. Therefore, the enzyme trapped in powder form is then solubilized inside the microcavity leading to a high density of biocatalyst in solution with an electrical connection with the buckypapers. The electrocatalytic performance of the bilirubin oxidase hollow electrode was described as a function of pH, temperature

Biography

Dr. Serge Cosnier is Emeritus Director of Research at CNRS at the Grenoble Alpes University (France) and professor at the Silesian University of Technology in Gliwice (Poland). His activity is focused on the molecular electrochemistry and bioelectrochemistry with the development of electrode materials whose applications include biological sensors and energy conversion. Dr. Serge serves as Editor of Bioelectrochemistry and Specialty Chief Editor of Frontiers in Analytical Chemistry and has authored over 410 publications. In 2013, Dr. Serge became a member of the Academia Europaea and was elected member of the European Academy of Sciences in 2019.

and the amount of entrapped enzyme. Owing to the complexity of optimizing a multienzyme system, this concept also constitutes an attractive strategy to design and optimize enzyme cascade reactions. Besides the easy modulation of enzyme ratios, we have also demonstrated the possibility of trapping with enzymes a redox mediator ensuring the electrical connection of an enzyme. On the other hand, the development of glyconanoparticles resulting from the self-assembly of block copolymers composed of polystyrene and cyclodextrin as an inclusion site will be also reported. These glyconanoparticles, which are stable in water, constitute a multivalent platform for binding hydrophobic fluorescent or electroactive molecules. These nanoparticles were applied to the elaboration of solubilized enzymatic fuel cell in solution or were grafted on surfaces for the development of amperometric enzyme electrodes.

Sergey Suchkov[1-6]*, Roger D. Kamm[9], Shawn Murphy[7,8], Arturo Solis Herrera[1], Holland Cheng[10]

[1]National Center for Human Photosynthesis, Aguascalientes, México

[2]Member, The Russian Academy of Natural Sciences, Moscow, Russia

[3]EPMA, Brussels, EU

[4]PMC, Washington, DC, USA

[5]ISPM, Tokyo, Japan

[6]AHA, Houston, TX, USA

[7]MGH, Boston, MA, USA

[8]Harvard Medical School, Boston, USA

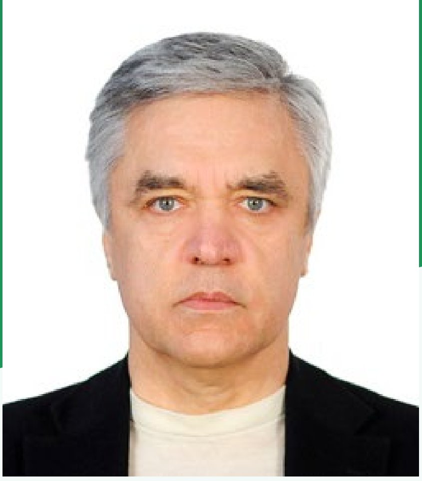
[9]MIT, Cambridge, MA, USA

[10]T College of Biological Sciences, UC Davis, CA, USA

Personalized and Precision Medicine (PPM) as a unique healthcare model through biodesign-inspired bio- and chemical engineering applications to secure the human healthcare and biosafety

A new systems approach to subclinical and/or diseased states and wellness resulted in a new trend in the healthcare services, namely, *Personalized and Precision Medicine (PPM)*. To achieve the implementation of PPM concept, it is necessary to create a fundamentally new strategy based upon the biomarkers and targets to have a unique impact for the implementation of PPM model into the clinical practice and pharma & medicinal chemistry bioindustry. In this sense, the translation of discoveries into

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 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: R&D Director of the National Center for Human Photosynthesis, Aguascalientes, México. The Russian Academy of Natural Sciences, Moscow, Russia. Member, New York therapies has not kept pace with medical need. It would be extremely useful to integrate data harvesting from different databanks for applications to provide more tailored measures for the patients and persons-at-risk resulting in improved outcomes.

Translational researchers, biodesigners, bio- and chemical engineers, and manufacturers are beginning to realize the promise of PP. Biodesign, bio- and chemical engineering, and nanobiotechnologies are being integrated into diagnostic and therapeutic tools to manage an array of PPM-guided conditions to customize therapeutic management. So, partnering and forming strategic alliances between researchers, bio-designers, bio- and chemical engineers, clinicians, business, regulatory bodies and government can help ensure an optimal development program that leverages the Academia and industry experience and FDA's new and evolving toolkit to speed our way to getting new tools into the innovative markets.

Healthcare is undergoing a transformation, and it is imperative to leverage new technologies to support the advent of PPM. It is urgently needed to discover, to develop and to create new (targeted and/or smart/intelligent) drugs being based on design-driven bio- and chemical engineering. With the support of nanotechnology, new targeted therapeutic agents and biomaterials, or aid the development of assays for disease biomarkers and identification of potential biomarker-target-ligand (drug) tandems to be used for the targeting, PPM is making phenomenal steps in the future to come.

Scaling up from a laboratory reaction to an industrial process is the main challenge for chemical and bioengineers resulting in the optimization at many levels. Moreover, developing and optimizing chemical and biotechnological processes plays a key role in modern society. This is the reason for developing global scientific, clinical, social, and educational projects in the area of PPM and design-driven translational applications to elicit the content of the new trend. The latter would provide a unique platform for collaboration among thought leaders and stakeholders

Academy of Sciences, USA. 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.

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. So, the Grand Change and Challenge to secure our Health and Wellness are rooted not in Medicine, and not even in Science! Just imagine WHERE?! In the upgraded Hi-Tech Culture!

Dr. Shree Niwas Chaturvedi

Centre for Aptitude Analysis and Talent Search,
Buxar, Bihar, India

Hot atom chemistry-past, present and future

Hot atom chemistry, a pivotal subfield of radiochemistry, investigates the chemical behavior of atoms with high kinetic energy produced during nuclear transformations. Since its inception in the mid-20th century, this field has provided profound insights into reaction mechanisms and atomic interactions under extreme conditions. Historically, the understanding of chemical effects induced by recoil atoms from nuclear reactions was instrumental in elucidating the behavior of radioactive isotopes, influencing nuclear fuel reprocessing and radiopharmaceutical development.

In the present era, hot atom chemistry finds applications in diverse domains. Advanced methodologies, such as pulse radiolysis and time-resolved spectroscopy, enable detailed kinetic studies of transient species formed in recoil processes. The field has also contributed significantly to targeted alpha therapy, where recoil atoms are utilized for precision oncology treatments. Additionally, the synthesis of novel materials through high-energy irradiation processes exemplifies its industrial relevance.

Looking ahead, the future of hot atom chemistry promises exciting directions. Emerging techniques in ultrafast spectroscopy and computational modeling are expected to deepen our understanding of high-energy atomic interactions. Integration with nanotechnology may lead to the design of innovative materials with applications in energy storage and catalysis. Furthermore, expanding the scope to environmental monitoring and sustainable nuclear technology underscores its role in addressing global challenges.

Biography

Dr. Shree Niwas Chaturvedi is a distinguished researcher, innovative educator, and advocate for transforming science education, earned Ph.D. in Chemistry, specializing in Nuclear and Radiochemistry, from Banaras Hindu University (BHU), Varanasi, in 2000. His pioneering research spans hot atom chemistry, the chemical effects of nuclear transformations, and energy conversion technologies. Soon after earning his doctorate, Dr. Chaturvedi established the Centre for Aptitude Analysis & Talent Search (theEXPLORER) in Buxar, India. This unique institute focuses on identifying and nurturing children's innate talents through aptitude-based analysis, equipping them to excel in their chosen fields. His teaching philosophy harmoniously blends ancient Indian educational wisdom with contemporary methodologies, creating an engaging and impactful learning environment. A prolific contributor to academia, Dr. Chaturvedi has authored numerous research papers, articles, and books. Highlights of his contributions include presenting "Water Splitting

This presentation will explore the transformative journey of hot atom chemistry, highlighting its historical milestones, current applications, and future potentials in advancing science and technology. The continued evolution of this field underscores its significance in modern scientific exploration and societal impact.

Technology for Efficient Thermal Energy Conversion" at the 4th Chemistry World Conference in 2024 and "Revolutionizing Science Education: Innovative Practices for Future-Ready Learners" at the World Education Conference in Athens, 2024. In 2025, he conducted a groundbreaking workshop on "Integrating Ancient Pedagogical Wisdom with Modern Educational Techniques for Holistic Learning" at the 8th International Conference on Future Education in Bali, Indonesia. Beyond research and education, Dr. Chaturvedi serves as a scientific advisor to Ganesh Engineering Works, Buxar, where he drives innovation in energy technologies. As an academic consultant to Heritage School and other institutions like Foundation School and Jawahar Navodaya Vidyalaya in Nawanagar, he empowers educators and students alike. Dr. Chaturvedi's contributions extend to community outreach through science seminars, teacher training workshops, and student enrichment programs. His relentless dedication to integrating innovative practices in education exemplifies his vision of equipping future generations with the knowledge and skills necessary to thrive in an ever-changing world. Recognized as a visionary leader, Dr. Shree Niwas Chaturvedi continues to inspire and revolutionize science education, leaving an indelible mark on the academic and scientific communities.

Silvia E. Asís*, Gisela C. Muscia

Universidad de Buenos Aires, Facultad de Farmacia & Bioquímica. Departamento de Ciencias Químicas Junín 956, Ciudad Autónoma de Buenos Aires, Argentina

Design and synthesis of nitrogen heterocycles with antileishmanial activity: From natural products inspiration to 2D/3D QSAR models

Leishmaniasis is a neglected vector-transmitted tropical disease caused by a protozoan parasites species of the genus *Leishmania*, where the three principal clinical manifestations are Cutaneous Leishmaniasis (CL), Mucocutaneous Leishmaniasis (MCL), and Visceral Leishmaniasis (VL). Known also as kala-azar, VL is fatal if left untreated in most cases. CL is the most common form of leishmaniasis and causes skin lesions, mainly ulcers, on exposed parts of the body, whereas MCL leads to the partial or total destruction of mucous membrane tissues. About 95% of CL/MCL cases occur in the Americas, the Mediterranean Basin, the Middle East, and Central Asia, with annually estimated 700 000 to 1 million new cases worldwide. The pharmacological treatment for leishmaniasis is limited, relying primarily on pentavalent antimonials, amphotericin B (under deoxycholate or liposomal formulations), and miltefosine. Additionally, these chemotherapeutic options are mostly unsatisfactory due to low efficacy, poor safety, the emergence of parasite resistance, among other factors related to treatment that are unsuitable for the socioeconomic reality of affected populations. Leishmaniasis chemotherapy has been historically associated with natural products, such as amphotericin B extracted from the filamentous bacteria *Streptomyces nodosus*, and paromomycin obtained from *Streptomyces rimosus*. Moreover, reports identifying natural products with antileishmanial activity are always

Biography

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

frequent. A series of 2-substituted quinolines isolated from *Galipea longiflora* K. Krause (*family Rutaceae*), a Bolivian tree traditionally used to cure ulcerations of CL by the native Chimanes tribe, was first reported by Fournet et al. Pure quinoline alkaloids, such as 2-n-propylquinoline, 2-n-pentylquinoline, 4-methoxy-2-phenylquinoline, and 2-(3,4-methylenedioxyphenyl-ethyl)-quinoline, demonstrated promising activity against *Leishmania donovani* (species related to VL) in vitro, and activity by oral route in the in vivo evaluation. This discovery encouraged us to develop C2-substituted quinolines as antileishmanial agents. In addition to their recognized activity as antimalarials, many synthetic quinoline derivatives are antibacterial, antifungal, antitumor, and antimycobacterial agents. We have previously reported the microwave-assisted synthesis of substituted 2-phenylquinoline-4-carboxylic acids and poly-substituted quinolines, which exhibited antiparasitic activities. Among them, four derivatives with moderate activity against *L. (Leishmania) infantum chagasi* and *L. donovani* were found. Furthermore, we have investigated the influence of the vinyl-bridge insertion between the 2-aryl ring and the quinoline core on the antileishmanial activity. Two derivatives possessing a 2-chloro or 4-chlorostyryl moiety, respectively, were considered the most promising antileishmanial agents due to the parasite killing effect in intracellular forms inside infected macrophages. In addition, it was demonstrated that certain chalcones can inhibit the growth of *Leishmania spp.*, such as the natural compound licochalcone and the synthetic derivative (E)-3-(3-nitrophenyl)-1-(2,4,6-trimethoxyphenyl)prop-2-en-1-one. In this context, we have developed two computational models based on Three-Dimensional Quantitative Structure-Activity (3D-QSAR) using Comparative Molecular Similarity Index Analysis (CoMSIA) and Two-Dimensional Quantitative Structure-Activity (2D-QSAR). Thus, a new series of twelve quinoline-chalcone hybrids was designed and synthesized, and the products were further evaluated against L. *(L.) amazonensis* to validate the model. Four compounds resulted active with IC50 values less than 2.61 M. These results suggest that the calculated models could be used for the rational design of new inhibitors with antileishmanial activity.

Stanislaw Dzwigaj

Sorbonne Université, UMR 7197, Laboratoire de Réactivité de Surface

Chemical engineering of vanadium, titanium or chromium zeolites for application in environmental catalysis

The vanadium, titanium or chromium ions well dispersed at zeolite framework could be considered as active sites of catalytic processes. So, the incorporation of these metals into zeolites as isolated tetrahedral sites appears to be the important task. We have earlier shown that the incorporation of transition metal ions into vacant T-atom sites of framework zeolite is strongly favored when, in the first step, zeolite is dealuminated by treatment with nitric acid solution and then, in the second step, the incorporation of transition metal ions results in the reaction between the cationic metal species of the precursor solution and the SiO-H groups of vacant T-atom sites created by dealumination of zeolite. During my keynote talk the chemical engineering of zeolites with vanadium, titanium or chromium ions will be described and characterized by different physical techniques both at the macroscopic (XRD, BET, TPR, TEM) and molecular level (FT-IR, NMR, DR UV-Vis, XPS, EPR, XAFS). The application of vanadium, titanium or chromium single-site zeolite catalysts in environmental catalysis will be discussed. This two-step postsynthesis method applied in this work allowed obtaining vanadium, titanium or chromium single-site zeolite catalysts active in different catalytic processes such as photocatalytic decomposition of NO, oxidation of 2-propanol into acetone and selective CO oxidation in the presence of H2 (partial oxidation (PROX) reaction).

Biography

Professor Stanislaw Dzwigaj received 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 Réactivité de Surface Université P. et M. Curie (Paris) obtained in 1990 a position of contracted researcher in the same Laboratory devoted to surface reactivity in relation to catalysis phenomena. Then, in 2008 obtained permanent position in CNRS as a researcher. On February 19, 2014 for outstanding scientific achievements, Professor Stanislaw received the title of professor and his published work includes more than 180 papers published in reputable international journals.

Theodosios Geo Douvropoulos

Hellenic Naval Academy/Physical Sciences
Sector, Piraeus Greece

Key chemical sensing applications of AlGaAs/GaAs heterostructures and a quantum resonant-tunneling based model thermometer

In this presentation, we propose a model thermometer based on resonant carrier transport in an AlGaAs/GaAs double-barrier heterostructure. We use a one-dimensional model to describe the effective potential of the heterostructure, which consists of two quantum barriers (AlGaAs layers) separated by a quantum well (GaAs layer). We consider the temperature dependence not only of the conduction band offset between the GaAs and AlGaAs layers, but of the effective mass of the carriers as well. The heterostructure is connected on both sides to two heavily doped GaAs layers, referred to as the emitter and the collector, where the carriers exist. When an external bias is applied between the emitter and the collector, the resonant tunneling mechanism is activated. This causes the disturbed energy levels of the quantum well quasi-states to align with the fermi level of the emitter, enhancing resonant tunneling. The complex energy disturbance of the quasi-states reveals both the real energy shift and the width of the resonance, with the latter providing the resonant transport time. By employing quasi-classical path integral theory, we can analytically derive the green's function of the heterostructure and calculate the resonance positions. These positions depend on various parameters, such as the geometry of the heterostructure, the applied bias, the aluminum mole fraction, and temperature. We calculate the resonant transport time as a function of the existing temperature. By inverting this relationship, we can obtain an accurate measurement of the heterostructure's temperature based on the resulting resonant time. Our results provide concise analytical relationships involving parameters such as barrier and well thickness, as well as shape, enabling the prediction and optimization of the performance of various nanoscale devices and particularly aiding in determining the required temperature for effective sensor

Biography

Dr. Theodosios Geo Douvropoulos studied Physics at Patra University, Greece (1996), then joined the research group of Prof. C.A. Nicolaides at the National Hellenic Research Foundation (Theoretical Physics and Chemistry Institute), where received a Master's degree in Physics (2001) and Ph.D. degree (2005) in "Resonant Quantum Dynamics". Dr. Theodosios's main research activity is about the quantum evolution of unstable low-dimensional physical and chemical systems. Has been published more than 25 research articles and has obtained the position of Senior Lecturer at the Hellenic Naval Academy of Greece since November 2022. Since 2023, Dr. Theodosios is the National Representative of Greece in NATO activities related to Quantum Technologies.

Thomas J. Webster

School of Health Sciences and Biomedical Engineering, Hebei University of Technology, Tianjin, China; School of Engineering, Saveetha University, Chennai, India; Division of Pre-college and Undergraduate Studies, Brown University, Providence, RI USA

Supramolecular nano chemistries: Fighting viruses, inhibiting bacteria, and growing tissues

Self-assembled, supramolecular chemistries were fabricated out of the DNA based pairs guanine and cytosine (G^C) to self-assemble into a rosette nanotubular structure when added to biological fluids through the formation of H-bonds in the x, y, and z directions. This presentation will cover the diverse promising medical (including tissue engineering and anti-viral) applications of rosette nanotubes. For tissue engineering applications, the rosette nanotubes have been well studied in vitro and in vivo for orthopedic, cartilage, wound healing, vascular, bladder and other medical applications. Rosette nanotubes (commercialized under the trade name ArxisTM) were injected into bone and cartilage defect sites and after 16 weeks and showed significantly new bone and cartilage growth compared to controls. In this manner, such materials may represent the future supramolecular chemistry for tissue engineering applications, replacing metallic orthopedic implants which currently have a failure rate of 5–10%. The rosette nanotubes have also been commercialized under the trade name Nx3TM for encapsulating and passivating numerous viruses in the body such as SARS-CoV-2 (which causes COVID), rhinovirus, influenza, and more. Specifically, in vitro studies using a transgenic mouse model demonstrated that after inhalation, Nx3TM reduced RNA in the lungs of SARS-CoV-2 infected mice similar to the control Paxlovid

Biography

Thomas J. Webster's (H index: 129) degrees are in chemical engineering from the University of Pittsburgh (B.S., 1995; USA) and in biomedical engineering from RPI (Ph.D., 2000; USA). Has formed over a dozen companies who have numerous FDA approved medical products currently improving human health in over 30,000 patients. His technology is also being used in commercial products to improve sustainability and renewable energy. Currently helping those companies and serves as a professor at Brown University, Saveetha University, Hebei University of Technology, UFPI, and others. Dr. Webster has numerous awards including: 2020, World Top 2% Scientist by Citations (PLOS); 2020, SCOPUS Highly Cited Research (Top 1% Materials Science and Mixed Fields); 2021, Clarivate Top 0.1% Most Influential Researchers (Pharmacology and Toxicology); 2022, Best Materials Science Scientist by Citations (Research.com); and is a fellow of over 8 societies. Prof. Webster is a former President of the U.S. Society for Biomaterials and has

(Pfizer) which is currently being used clinically to decrease COVID symptoms. However, unlike Paxlovid, COVID symptoms did not return after stopping Nx3TM treatment. In this manner, such materials may represent the future supramolecular chemistry for treating viruses.

over 1,350 publications to his credit with over 55,000 citations. He was recently nominated for the Nobel Prize in Chemistry. Prof. Webster also recently formed a fund to support Nigerian student research opportunities in the U.S.

Yong-Xiao Wang MD/PhD

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

Pharmaceutical chemistry studies of novel biologics and drugs for chronic obstructive pulmonary disease

Chronic Obstructive Pulmonary Disease (COPD) is a common and devastating lung disease with a high mortality. However, the current therapeutics for COPD are neither specific nor very effective. Moreover, the pathogenesis mechanisms for this disease remain largely unknown. COPD is well characterized by airway hyperresponsiveness and remodeling, thereby leading to airflow limitation. A very important player in airway hyperresponsiveness and remodeling in COPD is an increase in intracellular calcium ($[Ca^{2+}]_i$) in Airway Smooth Muscle Cells (ASMCs). $[Ca^{2+}]_i$ is well generated and controlled by multiple ion channels. In the current studies, we have started to explore which type of ion channels may mediate the increased $[Ca^{2+}]_i$ in ASMCs and COPD. Using the patch clamp recording, the Nobel Prize winners' technology, together with specific channel antibodies, we have found that type-3 canonical Transient Receptor Potential (TRPC3) non-selective cation channel, showed a predominant activity and expression among the entire TRPC channel family in ASMCs. Similarly, using the SMC promoter SM22α-driven TRPC3 channel shRNAs, we confirmed the predominant TRPC3 channel activity and increased $[Ca^{2+}]_i$ in ASMCs. This channel protein expression was significantly increased in COPD human ASMCs. The increased TRPC3 channel expression was highly correlated with ASM remodeling in COPD. In support, proliferation of human COPD ASMCs was abolished by the specific channel inhibitor Pyr3. Like Pyr3, TRPC3 channel gene Knockdown (KD) by its specific shRNAs also blocked the increased proliferation of COPD human ASMCs. In

Biography

Dr. Wang has been a Full Professor at Albany Medical College since 2006, had his MD, PhD and extensive postdoctoral training. Dr. Wang's research projects have been supported by numerous research awards from NIH, American Heart Association, American Diabetes Association, American Lung Association, and other agencies. And, 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. Moreover, Dr. Wang has served as the editorial board member, section editor, and the executive committee member and/or subcommittee chair.

contrast, TRPC3 channel gene overexpression produced an opposite effect. It is known that up to 90% of COPD are attributable to cigarette or e-cigarette smoking (CS or eCS), and nicotine is a most important biological component of CS and eCS. Indeed, nicotine inhalation induced airway hyperresponsiveness and remodeling in mice. These nicotine-induced responses were completely eliminated by intravenous injection of lentiviruses containing SMC promoter SM22α-driven mouse TRPC3 channel shRNAs using a hydrodynamic injection technique. TFSEARCH program predicts that the TRPC3 channel promoter region has the transcription factor NFκB binding sites. Thus, NFκB may mediate the increased TRPC3 channel expression and activity in COPD. Consistent with this view, nicotine significantly increased the activity of the transcription factor NFκB and the total expression levels of the key NFκB subunit p65 and p50 in human ASMCs. Moreover, both p65 and p50 expression levels were largely increased in the nucleus, but correspondingly decreased in the cytosol. Nicotine also largely increased TRPC3 channel promoter activity and this effect was blocked by the NFκB inhibitor Bay 11-7082. This NFκB inhibitor also blocked nicotine-induced TRPC3 channel mRNA expression in human ASMCs. Similarly, the NFκB subunit p65 and p50 gene KD produced a similar effect. Taken together, a series of our pharmaceutical chemistry studies have for the first time discovered that cigarette smoking or nicotine inhalation increases TRPC3 channel expression, channel activity, and $[Ca^{2+}]_i$ in ASMCs, thereby leading to airway hyperresponsiveness and remodeling (i.e., COPD). The increased TRPC3 channel expression and activity are attributed to the increased NFκB expression and activity in ASMCs. Moreover, TRPC3 channel and NFκB biologics and inhibitors may become novel and effective treatments for COPD.

5th Edition of

Chemistry World Conference

JUNE
02-04
2025

ORAL PRESENTATIONS

Amel S. M. Twfeek*, Yousif Sulfab

Department Department of Chemistry, College of Science, University of Khartoum,
P.O. Box 321 Khartoum

Inner sphere oxidation of 3,9-dimethyl-4,8-diaza-3,8-undecadiene-2,10-dione dioximecopper(II) complex by N-bromosuccinimide to copper (III) in aqueous acidic solutions

The kinetics of the oxidation of the 3,9-dimethyl-4,8-diaza-3,8-undecadiene-2,10-dionedioximecopper (II) complex, $[Cu^{II}HL_2]^{++}$, by N-bromosuccinimide (NBS) were studied in weakly acidic aqueous media (pH 3.36-5.25). The reaction exhibited autocatalysis, characterized by S-shaped absorbance-time curves. Under pseudo-first-order conditions in the presence of Hg (II), the reaction rate showed a first-order dependence on the total copper (II) complex concentration. The pseudo-first-order rate constant, k_{obs}, displayed Michaelis-Menten type saturation kinetics with respect to [NBS]. The dependence of k_{obs} on acidity was complex, increasing only by a factor of ~2 across the pH range studied. An inner-sphere mechanism is proposed, consistent with the derived rate law and the known ability of the four-coordinate $[CuIIHL]^+$ complex to form five-coordinate species. Considering $[Cu^{II}HL]^+$, $[Cu^{II}L]$, [NBS] and $[HNBS]^+$ as the reactive species within four possible pathways, the following rate law was derived:

$$\text{Rate} = \frac{\{k_1K_2K_3 + (k_2K_1K_2K_4+k_4K_6)[H^\pm] + k_3K_2K_5[H^\pm]_2\}[NBS][CuIILH^\pm]t\ (i)}{[H^+] + K_1 + \{K_1K_3 + (K_1K_2K_4 + K_6)[H^+] + K_2K_5[H_+]_2\}[NBS]}$$

Biography

Amel Salah is a researcher in food technology currently working with the Sudan Industrial Research & Consultancy Centre (IRCC) since February 2020, focusing on areas like food inspection and grading. She holds Master's degrees in Food and Beverage Innovation and Management from Università Politecnica delle Marche (Italy) and in Chemistry from the University of Khartoum (Sudan). With previous experience as a Teacher Assistant and Laboratory Technician, Amel is seeking opportunities in roles such as Researcher, Chemist, or Quality Control Specialist.

Arun K Shandilya*, **Anupam Shandilya**

Dr. H. S. G. University SAGAR

Discovery of helium in rocks of vindhyan super group around Sagar, South Ganga Basin, Bundelkhand Region M.P. India

Studies on the exploration of the helium gas in the rocks of the Vindhyan Super Group around Sagar, South Ganga Basin, Bundelkhand Region, M.P. is carried out in the detail with joint collaboration of Deptt. of Applied Geology and ONGC Energy Centre, Ahmadabad. As Author has already reported the Discovery of Helium has leakages through more than 50 tube wells/electric wells excavated in agriculture fields various villages in Sagar Distt. The geochemical analysis of the soil, gas and water indicates remarkable amount of helium gas in these tube wells, containing about 0.45 to 0.735 and methane varying from 72% to 99%. These investigations were done in the long research work (more than 25 years) dedication carried out in this area and research finding published in the Journal of National and International repute, which has attracted the officers/Scientists of ONGC, Dehradun, CGWB, Faridbad, Atomic Mineral Directorate Hyderabad and Bhabha Atomic Research Centre Mumbai.

The Result of the stable isotopic analysis of ethane gas in these samples δ C13 value are ranging from -24.9 per mill w.r.t. PDB and -26.9 per mill w.r.t. PDB and the methane gas are ranging from isotopic values -54.0-per mill w.r.t. PDB to -61.5 per mill w.r.t. PDB are indicative that this gas is of thermogenic origin, which must have been formed at very high temperature & pressure condition in the deeper horizon of the great vindhyan sedimentary basin of late proterozoic (>500m.y.) period. A reporting of leakages of above mentioned gas from 50 tubewells in the inliers of vindhyan rocks and even in the deccan trap rocks ensures that this area must be having a big gas reservoir within vindhayn rocks around Sagar-Distt. in M.P.

The ONGC energy centre Ahmadabad has started the detail collaborative geophysical work on the drilling exploration upto the depth of 600 m has been carried out and to be carried out in various location from where the leakages of has been earlier reported earlier. In these 600 m deep drill holes detail geophysical logging including the gama ray logging and neutron logging, lithological and structural logging will be carried out to know the probable gas reserve and at what depth the, we can get the gas for the exploration and utilization of these ases for industrial purpose and other uses etc.

The detail geophysical studies will be very much helpful in the gas reserve calculation and the depth of the gas pockes in the South Ganga Basin in Bundelkhand region in M.P.

Keyword: Vindhyan Rocks, Petroleum Gas, Helium, Proterozoic, Stable Isotopic, Geochemically, Leakages, Thermogenic.

Dr. Asish Bhaumik

Department of Pharmaceutical Chemistry, School of Pharmaceutical Sciences, Girijananda Chowdhury University, Tezpur-campus, Assam, India

Ionophores: Modulators of cellular ion homeostasis and emerging therapeutic agents

Ionophores are compounds that facilitate the transport of ions across cellular membranes, disrupting the normal ionic balance within cells. This disruption can lead to various cellular responses, including apoptosis (programmed cell death), making ionophores potential candidates in cancer therapy. Ion homeostasis is crucial for the survival of both normal and neoplastic cells. Disruptions in ion balance are characteristic of cancer cells, prompting the exploration of ionophores agents that modulate ion transport as potential anticancer treatments. Notable ionophores such as Valinomycin, Nigericin, and Obatoclax have demonstrated significant anticancer activities, particularly against cancer stem-like cells, which are often resistant to conventional therapies and contribute to tumor recurrence.

Keywords: Ionophores, Homeostasis, Neoplastic Cells and Anticancer Activities etc.

Biography

Dr. Asish Bhaumik is an Associate Professor in the Department of Pharmaceutical Chemistry at the School of Pharmaceutical Sciences (SOPS), Girijananda Chowdhury University (GCU), Tezpur, Assam, joined on March 15, 2023. He teaches courses such as Medicinal Chemistry, Pharmaceutical Organic Chemistry, Therapeutic Chemistry, Biochemistry, and Pharmaceutical Analysis. Dr. Bhaumik earned his Ph.D. in Pharmaceutical Science with a focus on Medicinal Chemistry from Assam Downtown University in 2022. He also holds an M. Pharm in Pharmaceutical Chemistry from The Tamil Nadu Dr. MGR Medical University (2012) and a B. Pharm from RIPSAT (2003). Additionally, he has graduate diplomas in Clinical Research and Applied and Industrial Biotechnology. Dr. Bhaumik has contributed significantly to pharmaceutical sciences through his authorship and patent holdings. He has authored textbooks such as "A Textbook of Pharmacology II (BP503T)" and "A Textbook of Pharmaceutical Biotechnology (BP605T)". He also holds two UK design patents and seven Indian patents, reflecting his innovative research in the field. In addition to his academic and research pursuits, Dr. Bhaumik has actively participated in national and international conferences, presenting papers and engaging with the broader scientific community. His dedication to continuous learning is evident through his attendance at various faculty development programs, quality improvement programs (18), short-term courses, and workshops (7) organized by reputed universities and institutions. Dr. Asish Bhaumik is currently supervising four Ph.D. scholars in the Department of Pharmaceutical Chemistry at the School of Pharmaceutical Sciences, Girijananda Chowdhury University (GCU), Tezpur.

Ayushi Rana

Forensic Science Department, Galgotias University/Assistant Professor, Greater Noida, Uttar Pradesh, India

Toxicological trend in Prayagraj, Uttar Pradesh, India

The topic includes the trends in poisoning cases across Prayagraj district—in Uttar Pradesh East India over a five-year period (2017-2021). The study provides a comprehensive analysis of poisoning trends through various dimensions, including yearly, gender-wise, area-wise, monthly, quarterly, seasonal, occupational, and marital status distributions. It also examines the type of poison involved and its relationship with demographic factors such as age. The statistical and percentage approach were used for the examination of these selected demographic parameters and this revealed that Prayagraj district reported the highest number of poisoning cases with 1,612 cases. the data showed a significant variation in poisoning cases across different times of the year, with the highest incidence observed in the summer months (June-August), accounting for 37.5% of the cases, and the lowest in the winter months (December-February), accounting for 22.3%. Gender-wise distribution indicated that males were more frequently affected, constituting 68.4% of the cases compared to 31.6% for females. Additionally, the study found that younger age groups (15-30 years) were most vulnerable, accounting for 45.8% of the cases, while older age groups (above 60 years) had the lowest incidence at 12.9%.

Biography

Ms. Ayushi Rana studied Life Science with a focus on Forensic Science at Sam Higginbottom University of Agriculture, Technology, and Sciences, Prayagraj, and graduated with a B.Sc. in 2019. She continued her studies at the same institution, earning a Master's degree in Forensic Science in 2019. Also submitted her Ph.D. thesis on the topic "Poisoning Trends Among Selected Districts of Uttar Pradesh East and Efficacy of Analytical Methods for Their Detection" at Sam Higginbottom University of Agriculture, Technology, and Sciences, Prayagraj, U.P. And, began her academic career as an Assistant Professor and Academic Coordinator at NIMS University, Jaipur, followed by roles as an Assistant Professor at Om Sterling Global University and Galgotias University, gained over 4 years of teaching experience. She has qualified the UGC NET Examination twice, once in June 2019 and again in December 2020. MS. Ayushi Rana vocational training includes experience at the Government Forensic Laboratory, Lucknow, Uttar Pradesh, where she received training in forensic science, forensic serology and biology, and forensic fieldwork with the Allahabad Police Crime Branch.

Bhaskar Chakraborty

Organic Chemistry Research Laboratory Sikkim Government College (An Extention Centre of Sikkim University) Gangtok, Sikkim–737102, INDIA

Green chemistry protocol for the synthesis of some new scaffolds of isoxazolidine & isoxazoline derivatives via 1,3-dipolar cycloaddition reaction and potential biological activities of the cycloadducts

One of the excellent examples of spin trapping reagents is nitrones which plays fundamental role in the synthesis of five-membered heterocyclic ring compounds (commonly called isoxazolidine and isoxazoline derivatives) via 1,3-dipolar cycloaddition reactions which are an integral part of many natural products. The medicinal activities of these heterocyclic compounds always finds a tremendous interest to the synthetic organic chemists as they found to exhibit antibacterial, anticonvulsant, antibiotic, antituberculer, antifungal and anticancer activities. Except green chemistry methodologies, majority of the reported procedures for the synthesis of isoxazolidine and isoxazoline derivatives require drastic experimental conditions like high temperature and long reaction times. In addition, these reactions found to suffer from selectivity and also there are possibilities of poor yields as well as development of side products. Majority of these conventional procedures for the synthesis of isoxazolidine and isoxazoline derivatives are replaced successfully nowadays with the inception of green chemistry procedures like mechanochemistry (solid phase reaction), reactions conducted “in water” & “on water”, microwave induced reactions and many more techniques. In the present work, few excellent examples based on stereoselective 1,3-Dipolar cycloaddition reactions using green chemistry protocols have been reported. Good to excellent yields, minimum reaction time, fast & simple isolation of products, environment friendly reaction conditions and stereoselectivities in the reported reactions will certainly attract researchers working in this domain.

Keywords: Stereoselective 1,3-Dipolar Cycloaddition Reaction, New Approaches, Green Chemistry Methodologies, Anticancer Activity.

Biography

Professor of Organic Chemistry at Sikkim Government College (An Extension Centre of Sikkim University), Gangtok, Sikkim, India with 30 years of teaching experience in teaching Undergraduate and Post graduate Chemistry students. Has active research experience of 30 years in synthetic organic chemistry in the field of “Nitrone cycloaddition reactions and their further applications following green chemistry methodologies”. Has established few environment friendly greener methodologies along with atom efficient reactions in the synthesis of few novel isoxazolidine and isoxazoline derivatives using new nitrones via 1,3-dipolar cycloaddition reactions. These novel isoxazolidine and isoxazoline derivatives are found to have vast synthetic potential as they could be used as precursor for the synthesis of a variety of new organic molecules including peptides with potential biological activities. Supervisor of research scholars leading to Ph.D degree for 24 years (Awarded 8 Ph.D scholars

& 2 are working). Has 21 years of administrative experience as “Head of Department” in the institution. Former “Overseas Fellow” at the Cardiff University, Cardiff, Unied Kingdom in 2019. Has sufficient expertise in conducting DST/CSIR/UGC national research projects. Has published 70 nos of peere reviewed research publications (Scopus & WOS) in international and national journals of high repute and impact factors. Honorary referee and editorial board member for reviewing research manuscripts for various international and national journals with good impact factors. Has authored two books on the “Synthetic applications of nitrone cycloaddition reactions”. Has been awarded with many international and national awards. Has been associated as “Life member” with various international and national scientific organizations. Has presented research papers in various international and national conferences as “Invited Speaker” in UK, Germany, Greece, France and India. Has performed activities as “Organizing Commettee Members” (OCM) in international conferences.

Brij Bhushan Tewari

Department of Chemistry, Faculty of Natural Sciences, University of Guyana, P.O. Box: 101110, Georgetown, Guyana

Metal complexes in biology and medicine: The system aluminum (III)/chromium (III)/iron (III)–norvaline

In coordination compounds studies, knowledge of the stability constants of complexes is necessary for preliminary quantitative treatment. Metal complexes can offer their action such as anti-inflammatory, antimicrobial, antibiotic, anti-thyroid and anticancer compounds. Metal based drugs bioactivity can be increased by metal chelation, which in turn increase their absorbance and stability. Recent advances in inorganic chemistry have made possible formation of number of transition metal complexes with organic ligands of interest which can be use as therapeutic agents. Aluminum prefers oxygen donor groups for complexation. The stability of complexes in biological systems depends on pH, which in blood plasma is 7.4. Chromium is a very adaptable metal, and it can form copious species with variable oxidation numbers from (-VI) to (+VI). Iron is a component of heme and chlorophyll and serves as micronutrient of plants and animals. Ferric ion from Industrial effluent has the potential to poison animals and plants. The present technique involving the use of paper ionophoresis is described for the study of equilibria in binary complex systems in solution. The method is based on the movement of a spot of a metal ion in an electric field at various pH's of background electrolyte. A graph of pH versus mobility was used to obtain information in the binary complexes and to calculate its stability constants. Using this method, the stability constants of binary complexes metal (III)–norvaline have been determined to be (8.73±0.03, 7.20±0.04); (9.00±0.01, 7.41±0.05); and (9.41± 0.01, 7.66±0.11) (logarithm stability constant values) for aluminum (III), chromium (III) and iron (III) complexes, respectively, at ionic strength 0.1 Mol/L and a temperature of 3^0C. The first and second stability constants of metal complexes follow the order Fe(III)> Cr(III)>Al(III).

Keywords: Paper Electrophoretic Technique, Overall Mobility, Metal Complexes, Stability Constants.

Biography

Dr. Brij Bhushan Tewari is a Professor in Chemistry in the Department of Chemistry at University of Guyana. Prof. Tewari obtained his Doctor of Philosophy degree in Sciences (Chemistry) from Allahabad University and Doctor of Medicine degree 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. Has been published 143 research papers in international journal, one book and 15 book chapters.

Carmen Kaiser Brügmann

XRF application Specialist Rigaku

The elemental analysis of granulated blast furnace slag using WDXRF for conformity as per the EN 197-1 international standard

Granulated blast furnace slag is made by rapid cooling of a slag melt of suitable composition, as obtained by smelting iron ore in a blast furnace and contains at least two-thirds by mass of glassy slag and possesses hydraulic properties when suitably activated. Granulated blast furnace slag shall consist of at least two-thirds by mass of the sum of Calcium Oxide (CaO), Magnesium Oxide (MgO) and Silicon Dioxide (SiO_2). The remainder contains aluminium oxide (Al_2O_3) together with small amounts of other compounds. The ratio by mass (CaO+MgO)/(SiO_2) shall exceed 1,0.

The WDXRF instrument was setup with the fusion calibration method for the accurate and precise oxide analysis of slag.

The slag needs to conform to the EN 197-1 International norm to be used as an extender in making CEMII Portland Slag cement, CEM III Blast Furnace cement and CEM V Composite cements.

In order to lower the carbon footprint and reduce CO_2 the clinker produced is used to produce more extended cements.

The kiln is fired with alternative fuels to make clinker that is more cost effective. The more alternative fuels used to make cement, the lower the carbon footprint X-ray fluorescence is used to show new ways of reducing CO_2.

Biography

Carmen worked for PPC Cement from the period of 2000 to 2019, as a Research Chemist then a Senior Chemist and as an XRF Specialist. Has 19 years of working experience. The work done at PPC cement entailed application support on all XRF instruments in the Group. Quality assurance is required at all production sites to be able produce accurate and reliable analytical data for process control. In order to achieve this, she ensured that sample preparation for all X-Ray Fluorescence (XRF) follows best operating practices, calibration curves on the XRF instruments are matrix matched and minerologcally representative of the materials used in the process. She conducted reviews on XRF, sample preparation and quality best operating methods throughout all PPC plants, ranging from inland, costal and International sites located in other African countries. Previous positions held have been as a Senior Chemist and later Research Chemist in the Chemistry Reference Laboratory at the ISO 17025 Accredited Group laboratory Operations. Her knowledge and vast experience is on working with various types of XRF instruments ranging from Energy Dispersive, Wavelength Dispersive, Sequential and Simultaneous Spectrometers. Carmen has extensive knowledge and experience in other analytical techniques including ICP-MS, ICP-OES, XRD, FTIR Ion Chromatography and general wet chemistry. Her problem solving skills and analytical knowledge in XRF spectrometry, wet chemistry analysis and sample preparation methods is key to providing much needed technical support to the Group on various different types of analytical equipment used for testing various materials in the cement industry. She also provided software support to the Group on the XRF instrument types, ranging from Thermo, PAnalytical, Bruker and Rigaku. She provided training (XRF spectrometry, wet chemistry and sample preparation best practices) to the Group Quality personnel. Carmen is a dedicated hard worker who pays attention to detail and possesses strong analytical skills. Currently Carmen is the XRF Application Scientist for Rigaku. The support is provided to International customer under the EMEA countries.

Chantale Njiomou Djangang[1*], Claudia Tchamo Leussa[1], Mamadou Yaya Bade[2], Jean Marie Kepdieu[1]

[1]Department of Inorganic chemistry, Faculty of Sciences–University of Yaoundé 1, Yaounde Cameroon

[2]Department of chemistry, Faculty of Sciences–University Gamal Abdel Nasser, Conakry, Guinea

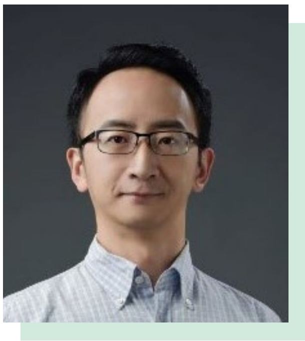
Use of industrial minerals to improve Portland cement's sustainability

Portland cement is the major industrial material that is manufactured commercially all around the world. It is used in construction of building, bridges, roads, and others structures. However, the production of this industrial material lead to the release of significant amount of CO_2 and greenhouse gas in the atmosphere. One tone of its production release about one tone of CO_2 gas in the atmosphere.

There is therefore a great need to look for actions that will transform this cement to an environmentally friendly material. Since last decade, the used of mineral materials such as Metakaolin as pozzolanic material in concrete and mortars have received considerable attention. Cameroon possesses rich sites of kaolinite clay and bauxite that are used mainly in ceramic. The use of these minerals in Portland cement manufacture will also be another contribution to fight again environmental pollution. This work investigated two industrial minerals (a gibbsite riched kaolin and a bauxite) that were used to partially replaced cement to elaborated mortars that were submitted to pozzolanic and mechanical tests. The pozzolanic results show that Cameroonian clay possesses the highest pozzolanic activity by chapel test. The mechanical strength shows that Cameroonian clay gives high compressive strength at young age, but at 28 days both of them give the same compressive strength. The study showed that pozzolanic properties of the two minerals greatly increased with heating up to at 600°C, and can also be used as ecofriendly supplementary cementitious materials in Portland for building construction.

Biography

Chantale Njiomou Djangang received Master's degree with thesis in chemistry (1995), Research Master's degree (2000) and a PhD degree (2007) in Materials Science all from the University of Yaoundé I. In addition, obtained a Teacher Training Certificate (1998) after two years at the Advanced Teacher's Training School of the same University. Chantale is a certified Master Teacher for Vocational Trainers and Program Development, having received training at KOREATECH, South Korea. Has teaching and research experience, progressively advanced through academic ranks at the University of Yaoundé I, serving from assistant in 2009 to Full Professor since 2022. Chantale work contributes in the constitution of data base on non-metallic minerals (clays, kaolin, laterite, limestone, feldspath rocks, pouzzolana, quartz and aggregates), their characteristics and transformation products. Has been Published 39 peer-reviewed articles.



Chaoyu Xiang

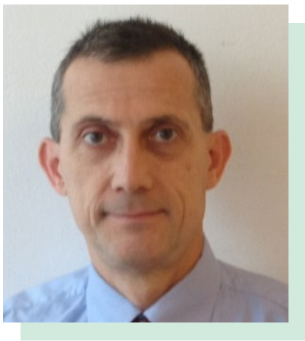
Ningbo Institute of Materials Technology and Engineering (NIMTE) of the Chinese Academy of Sciences (CAS)

Homogeneous nucleation and growth for synthesizing highly efficient and stable perovskite quantum dots and their light-emitting diodes

Lead halide chalcogenide nanocrystals are a promising light-emitting material for next-generation display technologies, capable of achieving near-100% photoluminescence quantum yield, narrow light-emitting spectra, and easily tunable light-emitting wavelengths. However, chalcogenide nanocrystals for light-emitting diodes are usually synthesised by difficult-to-control substitution reactions, resulting in low yields, inhomogeneous crystal growth and poor stability. To synthesized high-quality chalcogenide nanocrystals for use in chalcogenide quantum dot light-emitting diodes, we propose a synthetic strategy for uniform growth nucleation. This strategy achieves control of nucleation and growth during synthesis by simultaneously eliminating clusters that affect nucleation and suppressing overgrowth of Ostwald ripening, and synthesises chalcogenide nanocrystals with a narrow size distribution, fewer defects, and highly controllable size. Specifically, we avoided the generation of PbX_2 clusters by using Lewis acids and Lewis bases with relatively high dissociation coefficients as precursor ligands. After nucleation, a growth inhibiting reagent was added to the synthesis system, which also regulates the reaction equilibrium and passivates the nanocrystals. The photoluminescence quantum yield and stability of red and green chalcogenide nanocrystals were significantly improved by our synthesis strategy. Stable and efficient green and red lead halide chalcogenide nanocrystals were synthesised. The prepared quantum dot light-emitting diodes achieved an external quantum efficiency of 24.13% at 517/17 nm and 25.80% at 646/40 nm, and achieved pure red emission with 26.04% efficiency at an emitting wavelength and half-height width of 628/33 nm. The green chalcogenide light-emitting diodes operated at a brightness of 10,000 cd/m² with lifetime T50 reached a record 54 minutes, while the operational stability of the red chalcogenide LEDs was improved by a factor of 70, and the pure red chalcogenide quantum dot light-emitting diodes had an operational lifetime of 729 minutes at a brightness of 1,000 cd/m².

Biography

Xiang Chaoyu researcher graduated from the University of Florida, has worked for Apple Inc and Universal Display Corp. in the U.S.,CL Industrial Research Institute and Ningbo Institute of Materials Technology and Engineering (NIMTE) of the Chinese Academy of Sciences (CAS).He has long been engaged in the development of new light-emitting devices (OLEDs and QLEDs), and is a pioneering worker in the research of deep-blue quantum dots LEDs, and has repeatedly refreshed the QLED and chalcogenide LED devices' efficiency and operating life of the world records, enabling them to reach the threshold of industrialisation. The relevant research results were applied to the world's first 5-inch full-colour AM-QLED and 31-inch full-colour AM-HQLED prototypes, forming a series of core device preparation technologies with independent intellectual property rights. Has been published more than 50 SCI papers as the first author/corresponding author, and has granted more than 100 patents.



Davor Margetić*, Karla Bulava, Antonija Karakaš

Division of Organic Chemistry and Biochemistry, Laboratory for Physical Organic Chemistry, Ruđer Bošković Institute, Bijenička c. 54, 10000 Zagreb, Croatia

Mechanochemical synthesis of thioureas and guanidines

Guanidines are interesting molecules containing carbon surrounded by three nitrogen atoms, with unique structural characteristics that contribute to their remarkable physico-chemical properties. In particular, their high basicity (superbasicity) and ability to form hydrogen bonds set them apart from other organic compounds. Their physico-chemical properties make guanidines valuable functionality in various applications, including their use as neutral, organic catalysts or components of receptor functionalities in anionic sensors. Various guanidine derivatives are widely distributed in nature, and they have also been explored synthetically. Numerous synthetic routes and reagents have been employed for guanidine synthesis. Recently, mechanochemistry has been recognized as a sustainable, solvent-free alternative to conventional organic solution-based synthesis. This solid-state approach offers several benefits, such as eliminating solvents, reducing chemical usage, simplifying the experimental procedures, and shortening reaction times. Consequently, mechanochemical synthesis often provides higher reaction yields in more environmentally friendly conditions than solution synthesis. In this presentation, solution and mechanochemical methods for the synthesis of thioureas and guanidines will be presented and their efficiencies will be compared. Synthetic routes starting from aromatic amines, the preparation of isothiocyanates, followed by aromatic thioureas, and finally substituted guanidines will be discussed.

Biography

Dr. Margetić is head of the Laboratory for Physical Organic Chemistry of the Rudjer Boskovic Institute in Zagreb, Croatia and is a titular member of IUPAC Organic and Biomolecular Chemistry Division III. Studied at the Faculty of Chemical Technology, University of Zagreb, and continued his education in theoretical and physical organic chemistry (MSc and PhD) at the University of Zagreb. After nine years of post-doctoral research at the Centre for Molecular Architecture, Central Queensland University, Australia (Professors Warrener and Butler) he was promoted to the position of senior scientist. Dr. Margetić has published more than 130 articles, 18 book chapters and four books.

Demmouche Abbassia* Professor in Biology, Bouazza Sofiane, Hamri Dounia Douaa, Labadi Khaled, Ouhib Rachid, Oughilas Ahmed, Darnamous Racha Nassima, Khalloua Zine Charaf, Mai Hicham, Allam Affaf, Kheradji Fatima

Biotoxicology laboratory, Department of Biology, Faculty of Natural Sciences and life-Djillali Liabes University of Sidi Bel Abbes, Algeria

The antioxidant and analgesic effect of red and white ginseng on wistar rats

Ginseng is a perennial herbaceous plant from the Araliaceae family which belongs to the genus Panax, especially cultivated in Korea, ginseng is recognized for its general tonic effect, useful for invigorating the body of tired or weakened people, in particular due to its anti-inflammatory and antioxidant effects.

The present work is conducted to assess the importance of panax ginseng by evaluating its use in a targeted population, then determining the pharmacological and therapeutic properties of panax ginseng to study the antioxidant activity of ginseng and its impact on analgesic activity in male Wistar rats.

First, information on the nutritional, therapeutic and cosmetic uses of ginseng was collected from 66 questionnaires. The second step is to evaluate the biochemical potential of the hydro-ethanolic extract of red ginseng and the aqueous extract of white ginseng in vitro and their impact on the antioxidant activity by the DPPH method, then the evaluation of the effect of two variations of panax ginseng on peripheral analgesic activity in male Wistar rats that were injected with acetic acid to induce abdominal pain.

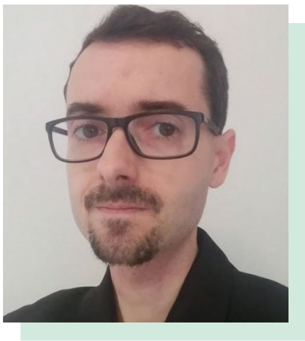
The investigation proved on the one hand, that ginseng is used as a treatment against: Depression, cardiovascular diseases and Diabetes. The antioxidant activity of the extract, by the DPPH method, showed that the red extract tested has a very high antioxidant potential, with an IC50 of 0.75 mg/ml. Comparison of white extract (IC50 of 6.03 mg/ml). The extract revealed a remarkable peripheral analgesic effect, Red Ginseng studied reduced the number of writhing from (46.7±10.0) to (12.3±5.0) with an inhibition rate of 73.66%. In addition, about the White Ginseng extract which has an inhibition rate of 66.8% with number of contrions (15.5±6.6).

To conclude, we can say that there is a significant difference between red and white panax ginseng, moreover it is main used for therapeutic purposes. Although the benefits of this product are well known, it is not yet widely used. The biochemical potential, without toxic effect, shows a good content in phenolic compounds due to the variability of these botanical origins which explains its considerable antioxidant capacity.

Keywords: White Ginseng, Red Ginseng, Analgesic Activity, Antioxidant Activity, Pharmacological Therapeutic.

Biography

Abbassia Demmouche studied biology at Djillaly Liabes University, Algeria and graduated as Engineer in 1999. She has received his PhD degree in 2009 at the same University. Currently, she is working as researcher in Djillaly Liabes University and she is a director of biotoxicology laboratory. She is serving as an editorial member of several reputed journals like journal of pregnancy & expert Reviewers for journals like « international research in medical and pharmaceutical sciences », « international journal of tropical disease and health ». She is a member in many International and National Medical Journals. He has authored many research articles and is an author on the subject of nutrition, epidemiology, anemia, pregnancy and Toxicology.



Ferran Acuña-Parés*, José Ignacio López Sánchez, Efrén Pérez Santín

Escuela Superior de Ingeniería y Tecnología (ESIT), Universidad Internacional de la Rioja (UNIR), Logroño, Spain

Disrupting TNF-α and TNFR1 interaction: Computational insights into the potential of D-Pinitol as an anti-inflammatory therapeutic

Tumor Necrosis Factor alpha (TNF-α) plays a critical role in the progression of inflammatory and autoimmune diseases by mediating pro-inflammatory pathways, making it a pivotal target for therapeutic intervention.1,2 D-Pinitol, a natural product with established anti-inflammatory and antioxidant properties, has been identified as a promising small-molecule inhibitor of TNF-α.3 Beyond its anti-inflammatory effects, D-Pinitol also exhibits antidiabetic, antioxidant, and anticancer activities, highlighting its broad therapeutic potential.1 This study employs an integrative computational approach, combining molecular docking, Discrete Molecular Dynamics (DMD), and Normal Mode Analysis (NMA), to investigate the inhibitory mechanism of D-Pinitol on the TNF-α/TNFR1 receptor complex.

Using a hybrid template-based and ab initio docking strategy, a model of the TNF-α/TNFR1 complex was generated. DMD calculations on the protein-protein complex identified three flexible regions with high binding potential for D-Pinitol, and docking studies and NMA simulations reveal that D-Pinitol preferentially binds within the central hydrophobic pocket of TNF-α. Specifically, D-Pinitol showed an enhanced binding energy for a distorted conformation of the protein complex and an increased number of stabilizing interactions for it, suggesting that D-Pinitol acts inducing significant structural distortions in TNF-α structure and disrupting its interaction with TNFR1.

This mechanism differs from traditional inhibitors, which often target the protein-protein interface. Comparative analysis with other natural product inhibitors, including EGCG and Japonicone A,4 highlights D-Pinitol's unique approach. By leveraging structural distortions and non-traditional inhibition pathways, D-Pinitol opens new avenues for targeting protein-protein interactions in cytokine-mediated disorders.

Biography

Dr. Ferran Acuña-Parés studied Chemistry at the Girona University, Spain, and graduated as MS in 2012, then joined the QBIS-CAT research group at the Institute of Computational Chemistry and Catalysis (IQCC) in the same university. Dr. Ferran conducted PhD studies under the supervision of Prof. Josep Maria Luis and Prof. Julio Lloret-Fillol, earning his degree in 2016. After one-year postdoc supervised by Prof. Julio Lloret-Fillol at the Catalonian Institute of Chemical Research (ICIQ), Spain, obtained the position of an Associate Professor at the Universidad Internacional de la Rioja (UNIR). Dr. Ferran has published 16 research articles in JCR journals.

Fu-Ming Tao

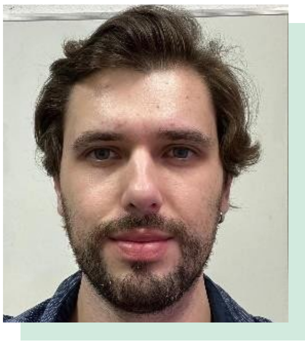
Department of Chemistry and Biochemistry, California State University, Fullerton, California 92834, USA

The chemistry of atmospheric smog and aerosols: Critical roles of ammonia

Oxides of nitrogen and sulfur are two major sources of air pollution, commonly known as Los Angeles (LA) smog and London smog, respectively. In this talk, I will briefly review prototype chemical reactions for the production of each type of smog. I will then show how a unique chemical species, ammonia, play a critical role in smog production as well as a possible solution of preventing smog in the atmosphere. Related to LA smog, we present a series of reactions involving three gases, NO_2, H_2O, and NH_3, to form Ammonium Nitrate (NH_4NO_3) aerosols and Gaseous Nitrous Acid (HONO). We attribute these reactions to be a significant source of atmospheric HONO responsible for the oxidation of all hydrocarbons and other organic compounds, leading to LA smog and ozone. In these reactions, ammonia is shown to play a critical role in lowering the Gibbs free energy barrier and stabilizing the Nitric Acid (HNO_3) product by forming particulate ammonium nitrate. Related to London smog, we present two series of contrasting reactions of SO_2, with and without NH_3. Once released into the atmosphere, SO_2 is shown react gradually with Water (H_2O), molecular Oxygen (O_2), and other species, converting into sulfate-based aerosols to form London smog. On the other hand, if NH_3 is added before SO_2 is released into the atmosphere, SO_2 reacts more readily to form ammonium bisulfate and ammonium sulfate solids. As a result, NH_3 may serve to prevent SO_2 from forming London smog. All reactions were studied by high-level quantum mechanical calculations with Dunning's augmented correlation-consistent basis sets. The M062X hybrid density functional method with the aug-cc-pVDZ basis set was used to determine molecular geometries, electronic energies, harmonic vibrational frequencies, and thermodynamic properties at stationary points of the potential energy surface. Single-point energy calculations were performed using coupled-cluster method with single, double, quadruple, and perturbative triple excitations, CCSD(T), with the aug- cc-pVDZ and aug-cc-pVTZ basis sets.

Biography

Dr. Fu-Ming Tao studied Chemistry at the University of Science and Technology of China and Suzhou University, and graduated as BS in 1982 and MS in 1985, respectively. Received PhD degree from Boston College in 1991. After postdoctoral work supervised by Professor Edward Mason at Brown University and by Professor William Klemperer at Harvard University, started a tenure-track faculty position at California State University Fullerton in 1995. Dr. Fu-Ming was promoted to Associate Professor with tenure in 2000 and Full Professor in 2005 and was a Henry Dreyfus Teacher-Scholar in 2000. Received research grants from different agencies including US National Science Foundation. Has been published more than 140 research articles in SCI (E) journals. The frequent citations of his papers have made him as the top 2% cited in the world list.



Gabriel Nicolai[1*], Harrson S. Santana[2], João L. da Silva Júnior[3], Osvaldir P. Taranto[1]

[1]School of Chemical Engineering, University of Campinas, Campinas, SP, Brazil

[2]Renato Archer Information Technology Center, Campinas, SP, Brazil

[3]Center of Engineering, Modeling and Applied Social Sciences, Federal University of ABC, São Bernardo do Campo, SP, Brazil

Comparative simulation of isopropyl palmitate synthesis in a microrreactor with static elements and a batch reactor

The personal care and beauty industry has significantly expanded in recent years. Within the variety of products encompassing skin, face, hair, and body care, oleochemicals stand out due to their animal or plant origin, which contributes to better sustainability compared to synthetic and petrochemical substances. One class of oleochemicals is fatty acid esters, which can be used as detergents, in cosmetics manufacturing, and in certain foods. Isopropyl Palmitate (IPP) is an oleochemical with adsorption properties, widely used in the personal care industry as an emollient and as an excellent organic solvent. To produce IPP, a variety of reactors are available, with the batch reactor being one of the most conventional and widely used in chemical and biochemical processes. However, it has certain disadvantages, such as limitations in homogeneity, thermal challenges, high energy consumption, difficulties in scaling up, among others. In this context, one alternative is the use of microreactors, as they have demonstrated numerous advantages due to fluid flow occurring at micrometric dimensions. This enables several benefits, including reduced residence time, low reagent consumption, low manufacturing cost, high heat and mass transfer rates, and a high surface-area-to-volume ratio. In many cases, simulations are performed prior to reactions, contributing to the identification of experimental starting points and process optimizations. Within the various branches of simulations, their application in chemical reactions has gained increasing prominence, as it allows for achieving higher yields, reaction conversions, and product selectivity. Routes to produce Isopropyl Palmitate (IPP) generally involve the esterification of palmitic acid with isopropanol in the presence of biocatalysts and high temperatures. However, a non-catalytic route at lower temperatures has emerged as an alternative to biocatalytic pathways and utilizes the following reagents: Palmitic Acid (PA), Thionyl Chloride (TC), and Isopropyl Alcohol (IPA). Initially, PA and TC react through a nucleophilic attack, forming PC and Hydrogen Chloride (HCl). In the second step, an alcoholysis reaction occurs in which IPA reacts with PC, forming a tetrahedral intermediate, which yields IPP. Therefore, the aim of this study is a comparison between simulations performed in a batch reactor and a microreactor with static elements for the synthesis of isopropyl palmitate. The simulations utilized kinetic data from a previous study conducted by other authors. In both reactors, the same conditions were maintained: temperature of 65°C and pressure of 1 atm. The results show that the batch reactor required 80–90 minutes to achieve a 99% conversion. Conversely, in the microreactor with static elements, a residence time of only 50 seconds was sufficient to achieve the same conversion percentage. The results show the distribution of reagents throughout their volumes. Therefore, it has been demonstrated that the use of microreactors with static elements is advantageous, as they enhance reagent mixing, enabling the production of the target compound with high conversions in significantly shorter times, compared to traditional reactors, which are still widely used in industrial processes.

Biography

MSc. Gabriel Nicolai studied Chemical Engineering at the Methodist University of Piracicaba–UNIMEP, Brazil, where graduated in 2018. Then joined the research group of Prof. Osvaldir Pereira Taranto at School of Chemical Engineering, University of Campinas–UNICAMP, and obtained MS in 2021. After that, began PhD in the field of microfluidics and isopropyl palmitate synthesis. Gabriel published one research article in Sage Journal, participated in conferences in Brazil and has recently submitted a book chapter on the importance of AI in microfluidics and a review research article on microfluidics in the field of personal care.

Kazuhiro Ishida
Matsugasaki 219-48, Kashiwa City, Chiba 277-0835, Japan

Multicenter molecular integrals over Dirac wave functions for solving the molecular matrix Dirac equation

The gauge-invariant matrix Dirac equation was derived by Yoshizawa [1] as given by

$$\begin{pmatrix} \overleftrightarrow{V} & \overleftrightarrow{T_m} \\ \overleftrightarrow{T_m} & \overleftrightarrow{W}-\overleftrightarrow{T_m} \end{pmatrix} \begin{pmatrix} \overleftrightarrow{C_-^L} & \overleftrightarrow{C_+^L} \\ \overleftrightarrow{C_-^S} & \overleftrightarrow{C_+^S} \end{pmatrix} = \begin{pmatrix} \overleftrightarrow{S} & \overleftrightarrow{0} \\ \overleftrightarrow{0} & \frac{1}{2m_ec^2}\overleftrightarrow{T_m} \end{pmatrix} \begin{pmatrix} \overleftrightarrow{C_-^L} & \overleftrightarrow{C_+^L} \\ \overleftrightarrow{C_-^S} & \overleftrightarrow{C_+^S} \end{pmatrix} \begin{pmatrix} \overleftrightarrow{\varepsilon_-} & \overleftrightarrow{0} \\ \overleftrightarrow{0} & \overleftrightarrow{\varepsilon_+} \end{pmatrix} \quad (1)$$

where $\overleftrightarrow{C_+^L}$ and $\overleftrightarrow{C_+^L}$ are the coefficient matrices for the large component spinor, $\overleftrightarrow{C_+^S}$ and $\overleftrightarrow{C_+^S}$ are those for the small component spinor, $\overleftrightarrow{\varepsilon_-}$ and $\overleftrightarrow{\varepsilon_+}$ are the energy matrices, $\overleftrightarrow{0}$ is the zero matrix, and the other matrix elements are given by

$$V_{\mu\nu} =< \chi_\mu | V | \chi_\nu > \quad (2)$$

$$(T_m)_{\mu\nu} = \frac{1}{2m_e} < \chi_\mu | \vec{\sigma} \bullet (\vec{p}+\vec{A}) \vec{\sigma} \bullet (\vec{p}+\vec{A}) | \chi_\nu > \quad (3)$$

$$(W_m)_{\mu\nu} = \frac{1}{4m_e^2c^2} < \chi_\mu | \vec{\sigma} \bullet (\vec{p}+\vec{A}) V \vec{\sigma} \bullet (\vec{p}+\vec{A}) | \chi_\nu > \quad (4)$$

and

$$S_{\mu\nu} =< \chi_\mu | \chi_\nu > \quad (5)$$

in which $\{\chi_\nu\}$ is a proper basis set, $\vec{\sigma}$ is the Pauli spin matrices, $\vec{p} = -i\hbar\nabla$ is the momentum $\vec{A}$ is the vector potential of the magnetic field due to the nuclear spin, and V is the scalar potential. We use the Gauss-type charge density distribution (GCDD) model [2] for the vector potential of the magnetic field due to the finite nucleus, because some experiments show that the nucleus is not the point charge but a finite nucleus [2] and the GCDD model is frequently used for several calculations [3-5]. We use the atomic units throughout the present report ($m_e = 1$, $e = 1$, $\hbar = 1$,$4\pi\varepsilon_0 = 1, c = 137.035999139$). However, we describe m_e, e, and $\hbar$ explicitly for the readers convenience when one converts the units to the natural units. Using the Dirac identity, we have

$$\vec{\sigma} \bullet (\vec{p}+\vec{A})\ \vec{\sigma} \bullet (\vec{p}+\vec{A}) = (\vec{p}+\vec{A}) \bullet (\vec{p}+\vec{A}) + i\vec{\sigma} \bullet (\vec{p}+\vec{A}) \times (\vec{p}+\vec{A}) \quad (6)$$

and

$$\vec{\sigma} \bullet (\vec{p}+\vec{A}) V \vec{\sigma} \bullet (\vec{p}+\vec{A}) = (\vec{p}+\vec{A}) \bullet V (\vec{p}+\vec{A}) + i\vec{\sigma} \bullet (\vec{p}+\vec{A}) \times V (\vec{p}+\vec{A}) \quad (7)$$

Equation (6) shows necessary physical quantities in Eq. (3). Equation (7) does those in Eq. (4). Equations (2)-(5) show all of necessary matrix elements for solving the Dirac equation.

Many researchers extend the matrix Dirac equation to the molecule [3-20]. For a molecule, the scalar potential may be the sum of one and two electron terms as given by

$$V = \sum_{iA} \frac{-2Z_A e^2}{\sqrt{\pi}\, r_0} F_0\left(\frac{r^2}{r_0^2}\right) + \sum_{i\,j} \frac{e^2}{r_j} \qquad (8)$$

where we use the GCDD model for the nuclear attraction. The Breit interaction [21] is not considered in the present report. Generally speaking, each matrix element is the multicenter molecular integral. It is natural to use the atomic Dirac wave function as the basis function for solving the molecular Dirac equation. However, there is no molecular integral formula for that purpose. The author derived the Gaussian-transform for the Dirac wave function centered at A in order to evaluate all of necessary molecular integrals as given by [22].

$$r_A^{-\varepsilon_A} \exp(-\zeta_A r_A) = \frac{\zeta_A^{1+\varepsilon_A}}{2\sqrt{\pi}\,\Gamma(1+\varepsilon_A)} \int_0^\infty ds\, s^{-3/2} \exp(-s\, r_A^2)$$

$$\times\left[\left(\frac{\zeta_A^2}{2s}\right)\int_0^1 dt\, \frac{(1-t)^{\varepsilon_A}}{t^{4+\varepsilon_A}} - \int_0^1 dt\, \frac{(1-t)^{\varepsilon_A}}{t^{2+\varepsilon_A}}\right] \exp\left(-\frac{\zeta_A^2}{4s\,t^2}\right) \quad (9)$$

where $\varepsilon_A = 1-\sqrt{1-(Z_A\alpha)^2}$ in which $\alpha = 1/137.035999139$ is the fine structure constant $\zeta_A = Z_A$ and in which $Z_A e$ is the nuclear charge. This Gaussian-transform is the only one formula to be able to evaluate the multicenter integral over Dirac wave functions. Using the formula, we can derive all necessary molecular integrals for solving the Dirac equation. Such will be presented in the conference.

Biography

Dr. Ishida joined the research group of Prof. Teijiro Yonezawa at the Kyoto University in 1970. Received PhD degree in 1975 at the same university. After one year postdoctoral fellowship supervised by Prof. Keiji Morokuma at the Rochester University, New York, obtained the position of a lecturer at the Science University of Tokyo. He was retired from the university in 2011. Dr. Ishida has been published more than 30 articles in science journals. For example, most important three articles are listed below: 1. K. Ishida, “Core radial polarization and the contact hyperfine structure of 4S state of nitrogen”, Phys Rev A12 (1975) 1153-1158. 2. K. Ishida, “Calculus of several harmonic functions”, J Comput Chem Jpn. Int. Ed. 8 (2022) 2021-0029. 3. K. Ishida, “Gaussian-transform for the Dirac wave function and its application to the multicenter molecular integral over Dirac wave functions for solving the molecular matrix Dirac equation”, IgMin Res. November 04 2024; 2(11): 897-914.

Kundan Sharma

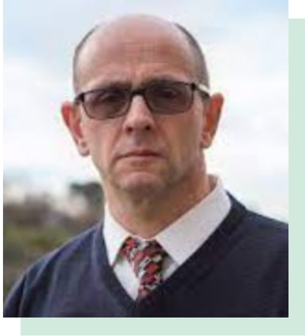
Department of Chemistry, Govt. College Nagrota Bagwan, Kangra, Himachal Pradesh, India

Indigenous technologies to check food adulteration: A native approach

Food adulteration poses significant health risks globally. This study explores and documents indigenous technologies employed by native communities to detect and mitigate food adulteration. By examining traditional knowledge systems, this research aims to highlight the efficacy and sustainability of native approaches in ensuring food safety. This study examines the traditional knowledge of indigenous communities regarding food adulteration detection. Employing ethnographic research and participatory observation, the research documents and analyses native techniques for identifying adulterants in commonly consumed foods. The study aims to validate the effectiveness of these indigenous technologies through a scientific lens and explores their potential for integration into modern food safety practices, thereby promoting culturally sensitive and sustainable food security.

Biography

Dr. Kundan Sharma is an accomplished academic and researcher specializing in physical chemistry, particularly related to surfactant solutions with amino acid and polymers and their application in pharmaceuticals and food industries. He has an extensive educational background, holding a Ph.D. in Chemistry from Himachal Pradesh University, Shimla and numerous accolades, including a selection in postdoctoral fellowship in Finland. Has been awarded for his research and contributions, including the DST Young Scientist grant to visit University of Regensburg Germany. Dr. Kundan has published 22 peer-reviewed articles in reputed journals, focusing on surfactant interactions and their thermodynamic properties. Has written 3 books on Physical Chemistry and Basic analytical chemistry.



Luca Vattuone

DIFI University of Genoa and IMEM-CNR, Genoa, Italy

H_2 dissociation at Ni(111) supported single-layer graphene

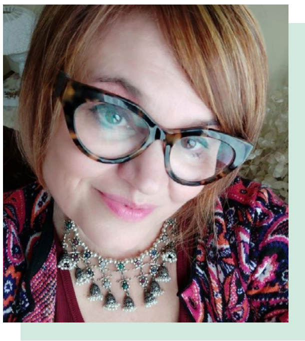
Adsorption and surface reactivity of 2D Materials such as graphene and h-BN is essential to understand at the fundamental level their sensing and catalytic properties as well as their functionalization. The interaction with the support is an important and not usually considered factor in applications. To study the effect of the substrate (Ni(111) in the present study) on the adsorption of H_2 single layer graphene is grown on Ni(111) by exposure to C_2H_4. Adsorption at room temperature (RT) in the mbar range is monitored by Near Ambient Pressure (NAP) XPS in beamtimes at Soleil and PSI Light Sources. Inspection of in-operando spectra shows that H_2 can dissociate on graphene on Ni(111) when exposure is performed under NAP conditions with H_2 pressure in the mbar range, i.e. significantly lower than for free standing graphene. Theoretical DFT calculations show that this is possible thanks to a substantial reduction of the activation barrier in presence of the Ni substrate.

Moreover when graphene coexists with NiO patches, an even higher H coverage is attained under the same conditions.

The strong interaction with the Ni(111) substrate substantially increases the reactivity of single layer Graphene with H_2 paving the way to the use of supported 2D materials as active supports and possibly even as catalysts.

Biography

L.V. got PhD in Physics at the University of Genoa in 1994. After a post-doc stay at the University of Cambridge (UK) with Sir D.A. King, then returned to Genoa. Since 1999 Luca Vattuone is a staff Researcher at Unige, and since 2012 Associate Professor of Condensed Matter Physics. His research interests cover adsorption at surfaces, self-assembling and surface reactions as well as surface plasmon dispersion and energy harvesting at surfaces.



Maria Cristina Gamberini

Department of Life Sciences, University of Modena and Reggio Emilia, Modena, Italy

Pharmaceutical polymorphs: Advanced strategies for solid-state characterization and optimization

The solid-state form of active pharmaceutical ingredients (APIs) exerts a decisive influence on critical quality attributes such as bioavailability, stability, and manufacturability. Among these, polymorphic transitions are particularly pivotal, as distinct crystalline modifications can exhibit divergent physicochemical behaviors, thereby necessitating rigorous analytical control throughout the drug development lifecycle.

This presentation delves into advanced methodologies for the comprehensive elucidation of pharmaceutical polymorphs, spotlighting Raman spectroscopy as a cornerstone in solid-state characterization. Owing to its intrinsic sensitivity to molecular vibrations and non-destructive nature, Raman spectroscopy provides unparalleled insight into lattice dynamics and intramolecular interactions, enabling precise differentiation between polymorphic species—even in complex matrices and at minimal sample volumes.

Additionally, the strategic deployment of Raman mapping allows for the spatial resolution of polymorph distribution within solid dosage forms, offering critical insights into heterogeneity and phase purity. The regulatory ramifications of these analytical advancements are equally substantial, as precise polymorph identification underpins intellectual property (IP) protection and ensures compliance with increasingly stringent quality guidelines.

Case studies presented herein will underscore the operational synergy between Raman spectroscopy and complementary techniques in unraveling the complexities of polymorphic systems, underscoring its role as a linchpin in contemporary pharmaceutical crystallography.

Biography

Dr. Maria Cristina Gamberini is a professor at the University of Modena and Reggio Emilia, specializing in pharmaceutical chemistry, crystallography, and nanomaterials. She holds a degree in Chemistry and has conducted research at the École Polytechnique Fédérale de Lausanne (EPFL, Switzerland) in nanomaterials and spectroscopy. With over 66 scientific publications and an H-Index of 26, Dr. Gamberini actively collaborates in the fields of nanotechnology, solid-state chemistry, and pharmaceutical analysis, focusing on crystallographic methodologies for drug development.

Mausul Umar[1*], Amina Doho[1], Abdurrahman Abubakar[1], Sani Shuaibu Kafin Hausa[2]

[1]Department of Chemical Sciences, Federal University of Kashere, Gombe, Nigeria

[2]Department of Biology, Khadija University Majiya, Jigawa State, Nigeria

Application of biochar for the removal of cadmium from industrial waste

The growing levels of cadmium (Cd) in environmental contexts substantially threaten public health and ecosystems. This research explores the effectiveness of biochar produced from agricultural waste as a sustainable material for capturing cadmium ions from industrial wastewater by employing batch adsorption experiments conducted under controlled laboratory conditions. The experimental factors considered were contact time, initial cadmium concentration, pH, and biochar dosage were meticulously analyzed. The findings revealed a swift adsorption process, achieving over 85% cadmium removal in just 65 minutes. The optimized pH for optimal cadmium adsorption was determined to be 7.0, which minimized competitive ion interactions. The adsorption equilibrium was described by both Freundlich and Langmuir isotherm models, with Langmuir demonstrating a more accurate fit ($R^2 = 0.9569$), suggesting the presence of monolayer adsorption on a surface with a limited number of identical sites. Kinetic studies indicated that the adsorption followed a pseudo-second order model, highlighting the significance of chemisorption due to the high equilibrium adsorption capacity values (qe) ranging from 3.709 to 7.880 for pseudo-second order compared to 6.720 for pseudo-first order. Conclusively, this shows that biochar is a viable and sustainable substrate that can be efficiently utilized for combating cadmium contamination in industrial waste streams. Thus, enhances environmental conservation and resource recovery initiatives.

Keywords: Cadmium, Biochar, Adsorption.

Biography

Mausul Umar studied industrial chemistry at Bayero University Kano Nigeria in 2012 and proceeded to Eastern Mediterranean University Cyprus for Master of Science in chemistry which he finished in 2017. Currently working at Department of Chemical Sciences, Federal University of Kashere, Nigeria which Umar joined in 2018. Has been published a book and more than ten research articles and received many certificates for conferences and webinars.

Michael Anjello Jothi Rajan[1*], K.Pandiyan[2]

[1]Associate Director, KNK Renewables, Bengaluru, Karnataka, India

[2]Professor and Head, Department of Inorganic Chemistry, Guinfy Campus, University of Madras, Chennai, India

Improving chemistry education with special reference to India

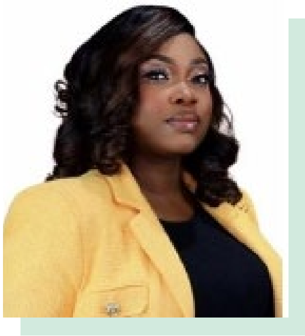
There are nearly 2904 colleges that offer Under Graduate Course in Chemistry in India. Out of these 2904 Chemistry colleges in India , there is a split of colleges by ownership, private: 985, public / government: 704 & public private: 518. This is the available statistics for the year 2023-2024. But there is a considerable decrease in class room strength in many of the UG Colleges in Tamil Nadu State in India for which no concrete reason is known. In the authors' opinion the non-science courses offer the students a nice platform to enter into the job market as new jobs are created in AI, IT, Business Administration, Commerce etc.,
Also it is a sad to know a good population of Higher Secondary Students are not willing to take the traditional Science Courses for their under graduate degree.

In this presentation the authors probe into the possibilities to increase the positive impact Chemistry teaching in Higher Secondary Courses and under graduate Chemistry course with a modified ROPES Model which may suit teaching of Science Subjects.

Keywords: Chemistry Education - Highere Secondary - Under Graduate - ROPES model.

Biography

Michael Anjello Jothi Rajan, Ph.D., Doctorate in Physics, (Ph.D., Physics), had retired from active service on 31.05.2017 having worked as an Associate professor of Physics; Director, Bio-Nano Research Laboratory and Dean of Research and Projects in Arul Anandar College (Autonomous), Karumathur – 625514, India. At the same time, he was heading the Department of Foundation Courses for a period of 13 years obtaining projects from UGC, New Delhi.
He is in the editorial board and reviewer board for many national and international journals. He is in the Technical Advisory Committee for many International Conferences in the field of CANCER THERANOSTICS. He served as the PROJECT CONSULTANT in the prestigious Tamil Nadu State Council for Science and Technology, Chennai, Tamil Nadu, INDIA from December 2017 to December 2020. At present he serves as Associate-Director, Anantharaman Applied Research Centre for Science & Technology Innovations for Villagers Livelihood Empowerment, Don Bosco College (Co- Ed.), Athanavur, Yelagiri Hills, Tamil Nadu Pin: 635853, Tirupattur District, Tamil Nadu, INDIA since December 2022.



Oluchukwu Aloke[1*], Alex Nelson[1], Erin Temple[2]

[1]Production Chemistry, SLB, Aberdeen, Scotland, United Kingdom

[2] Production Chemistry, SLB, Stavanger, Rogaland, Norway

New scale dissolver for the removal of elemental metal deposits

The formation and deposition of mineral scales during energy production is a well-known issue in the oil and gas industry as well as the geothermal sector. Mineral scales can cause several issues ranging from formation and equipment damage, production delays, to loss of time and resources leading to expensive remedial solutions. The use of chemical scale dissolvers in dissolving oilfield scale is a well understood concept which is widely researched and implemented. While some mineral scales can be seen as easy to dissolve especially for acid soluble scales like calcite, some mineral scales are more challenging to remove once formed. One of these types of scale is elemental metal deposits like lead which forms as a thin layer on equipment and tends to be radioactive due to the transportation of lead-210 (210Pb) radioisotope from the reservoir to the surface. Radioactive metal deposits present additional safety risks and environmental restrictions in their removal and handling. There are currently limited dissolvers specifically designed for the safe removal of radioactive lead so acid dissolvers are typically used.

This work focused on the evaluation of a newly developed scale dissolver designed primarily for dissolving radioactive lead deposits under surface and downhole temperature conditions applicable to both oil and gas and geothermal environments. Static soak tests were performed in the lab using lead shots at 20 - 22°C and 160°C respectively. The corrosivity of the dissolver against various metals, elastomers and thermoplastics commonly used in the oilfield was also evaluated. The dissolution results showed that at 20 - 22°C, the dissolver with the addition of <10% of hydrogen peroxide as a catalyst, can dissolve metallic lead up to 10grams per liter and up to 31grams per liter at 160°C without the addition of a catalyst. The rate of dissolution was also tracked at 20 - 22°C within a 24-hour period, which showed that 18% of a 1-gram lead shot sample had dissolved within the first 2 hours.

Biography

Oluchukwu obtained a degree in Industrial Chemistry from Enugu State University Nigeria in 2006, then completed a masters in Instrumental Analytical Sciences specializing in Oilfield Chemicals from Robert Gordon University, Aberdeen, Scotland in 2011. Oluchukwu has gained over 15 years work experience as a chemist working in the oil and gas industry mainly on research, product development and sustainability projects. She currently works as a senior chemist within the flow assurance team in SLB providing chemical solutions to mineral scale challenges in the oilfield.

Pengju Wu*, **Yangxian Liu**

School of Energy and Power Engineering Jiangsu University, Zhenjiang, Jiangsu, China

Current research progress in heavy metals poisoning of Selective Catalytic Reduction (SCR) denitration catalysts

Selective Catalytic Reduction (SCR) technology is the most extensively used and efficient method for NOx removal owing to its high removal efficiency and environmentally friendly process. However, heavy metals that are present in flue gas can deactivate the SCR catalysts through poisoning their active sites, leading to performance deterioration. To address this challenge and reduce the operating costs of SCR systems, it is essential to investigate the mechanisms of heavy metal poisoning and develop effective strategies to mitigate its impact. We reviewed the current research progress of the poisoning mechanism of different heavy metals on SCR catalysts (including vanadium-based catalysts, manganese-based catalysts, cerium-based catalysts). Various anti-heavy metal poisoning measures and mechanisms (e.g., doping metal and non-metal elements, etc.) were summarized. Research indicates that heavy metal deposition on SCR catalysts leads to pore blockage, reducing the catalyst's specific surface area and pore volume. This will damage to the active sites on the catalyst surface, which results in the physical and/or chemical poisoning of catalyst, thereby reducing the catalyst performance. Strategies to enhance the anti-poisoning capabilities of SCR catalysts include doping with metals or non-metals and the development of advanced carrier materials. Besides, the regeneration measures of SCR catalysts poisoned by heavy metals were also reviewed. Thermal reduction method, solution wet washing and composite method are the common methods for the regeneration of heavy metal-poisoning SCR catalysts. In the end, the main conclusions and research suggestions for the development of heavy metal poisoning of Selective Catalytic Reduction (SCR) denitration catalyst were also commented.

Biography

Mr. Wu is a PHD student majoring in thermal engineering at the School of Energy and Power Engineering, Jiangsu University, China. Mainly engaged in the research of coal-fired flue gas pollutants removal using biochar adsorption.

Peron Bosco Leutcha[1,2]*, Moïse Sirlam[1], Humaira Zafar[2], Muhammad Iqbal Choudhry[2], Alain Meli Lannang[3]

[1]Department of Chemistry, Faculty of Science, University of Maroua, Maroua, Cameroon

[2]H.E.J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi, Pakistan

[3]Department of Chemical Engineering, School of Chemical Engineering and Mineral Industries, Ngaoundere, P.O. Box 454, Cameroon

Flavonoids and other metabolites from the leaves of *Garcinia smeathmannii*, *in vitro* and *in silico* anti-inflammatory potentials

Garcinia smeathmannii is a well-known plant for its uses in the effective treatment of intestinal parasites, skin eruptions and skin burns. The dichloromethane-methanol (2:3) crude extract of the leaves of G. smeathmannii led to the isolation and characterization of twenty compounds (1–20) using chromatographic and spectroscopic techniques. Extracts and compounds were screened in vitro for their anti-inflammatory (ROS), antiglycation and antileishmanial (L. tropica) activities. Compounds were also screened for their *in silico* anti-inflammatory activities using Maestro 4.2.1 software with the co-crystal complex structures of the ovine oCOX-1: meloxicam (PDB Id: 4O1Z) and murine mCOX-2: meloxicam (PDB Id: 4M11) proteins. An unprecedented flavonol [6,8-C-dimethylkaempferol 4′-acetate 3,7-dimethyl ether (1)] and a flavone dimer [4′,7″-diacetylamentoflavone (2)] together with eighteen known compounds sorted as three biflavones [amentoflavone (3), sequoiaflavone (4)and, a mixture of sequoiaflavone (4) and putraflavone (5)], one ceramide [citropremide (6)], two alkylphenols [eugenol, 1 acetate (7) and eugenol (8)], two benzoic acids [diisooctyl phthalate (9) and anhydride benzoic (10)], one glucoflavone [vitexin (11)], two xanthones [1,2,5-trihydroxyxanthone (12) and 1,3,6-trihydroxyxanthone (13)], one triterpène [D:Afriedoolean-6-ene (14)], two sterols [a mixture of stigmasterol (15) and *β*-sitosterol (17)], two sterol glucosides [a mixture of stigmasterol glucoside (16) and β-sitosterol glucoside (18)], and two fatty acids [dotriacontanoic acid or lacceric acid (19) and tritriacontanoic acid or psyllic acid (20)] were characterized. All the tested samples in vitro revealed no antiglycation and antileishmanial activities. Beside, extracts revealed moderate anti-inflammatory activities (IC50 ranging from 24.1 ± 2.0 to 34.7 ± 0.8 µg/mL). Only compound (13) revealed an anti-inflammatory activity which was 9.33 times more active than the reference (Ibuprofen, IC50 = 11.2 ± 1.9 µg/mL) with IC50 of 1.2 ± 0.0 µg/mL. Compounds (2–9, 11–13 and 19–20) were docked and the docking scores were ranging from −10.178 to −6.119 (kcal/mol) which were in agreement with the experimental anti-inflammatory activity. These results are in agreement with the traditional uses of the leave of *G. smeathmannii* as cataplasm for skin eruption and as analgesic agent.

Biography

Dr. Peron Bosco Leutcha (PhD) studied Chemistry at the Dschang University, Dschang and graduated as MS in 2015. He then joined the Natural Products and Environmental Chemistry Research Group (NAPEC Research Group) headed by Prof. Dr. Alain Meli Lannang at the Higher Teacher Training College of the University of Maroua. He received his PhD degree in 2021 at the same institution. After six months TWAS-ICCBS postdoctoral fellowship supervised by Prof. Dr. Muhammad Iqbal Choudhry at H.E.J. Research Institute of Chemistry, International Center of Chemical and Biological Sciences (ICCBS), University of Karachi, Pakistan. He has published more than 23 research articles in SCI (E) journals.

Prof. Dr. S. Nawazish Mehdi*, Mr. B. Sunderlal Naik, Dr. S. Irfan Sadaq

Osmania University, India

Improved performance and reduction in engine emissions by the use of chemical mixture of turmeric leaf oil and diesel blends

In the contemporary world, the rapid depletion of fossil fuels has heightened the demand for alternative fuels. Research is being performed globally to identify biofuels as substitutes for conventional fossil fuels. The automotive industry has expanded significantly, necessitating improved performance of internal combustion engines. The demand for alternative fuels has escalated to meet the requirements of automobile compression ignition engines, including enhanced efficiency and reduced emissions.

The present work is aim to study the performance characteristics of Variable Compression Ratio (VCR) engine using 17.5:1, 18.5:1 and 19.5:1 as the compression ratios with diesel and Turmeric Leaf Oil (TLO) and their blends as biofuels by applying various loads as 5 kgs to 9 kgs. Parameters such as percentage of TLO mixed with diesel, load applied and compression ratios are considered in performing the test on VCR engine to determine their brake thermal efficiency, volumetric efficiency, specific fuel consumptions and emissions such as CO, CO_2, O_2 and unburnt hydro carbons. From the results it is concluded that kinematic viscosity increases from 1.62cSt to 2.88cSt at 43.75% from TLO to B70 blend. When compared between pure diesel and B70 blend, B70 attained 14.79% lower value than pure diesel. Fire point of pure diesel is 70°C and B70 has 72°C which is 2.77% higher than pure diesel. And the similar values are attained to the flash point. These values indicate that the biofuel namely TLO blend B70 can be used as an alternative fuel in diesel engine, based on the encouraging results obtained for the above said engine performance parameters.

Keywords: Turmeric Leaf Oil (TLO), Blends, Centistoke (cSt), Variable Compression Ratio (VCR) Engine, Emissions.

Biography

Dr. S Nawazish Mehdi is a distinguished Academician and researcher with over 40 years of teaching experience. He has held various key positions, including Principal Investigator for AICTE Research Projects, Ex-DEAN, Ex-HOD, and Ex-Director of R&D. Currently, he serves as a Ph.D. supervisor at Osmania University, JNTUH, Mewar University, and Singhania University. His expertise and influence extend beyond academia as a Member of the Board of Studies for JNTUH (Energy Studies), LIET (A), and several other institutions. Dr. Mehdi's contributions to research are significant, particularly in the field of IC engines and renewable energy & sustainable engineering and automobiles. He was awarded many funded research projects from Government, Ex: A ₹6 Lakhs research grant by AICTE under the R&D Scheme (2002-03) for his project on "Design Modifications in IC Engines to Use Hydrogen Fuel," with the completion report submitted in April 2006. He has also led various innovative projects funded by the A.P. State Council of Science & Technology, including Solar Electric Cars, Hybrid Vehicles, Regenerative Braking Systems, and Variable Compression Ratio (VCR) Engines. A prolific researcher, Dr. Mehdi has guided more than 12 Ph.D. candidates and is currently mentoring 7 others. His academic contributions include over 90 publications in international and national journals and conferences. Additionally, he has authored four textbooks, had two patents granted, and one patent recently published. He has also served as a reviewer for numerous Scopus and Web of Science-indexed journals, further solidifying his position as a thought leader in engineering research. Dr. Mehdi's dedication and achievements have earned him several prestigious awards, including the Outstanding Researcher Award (2024) from IEOM Society International, the Engineering Seva Ratna Award from ECIF, a gold medal from the Madina Education Society, and the Life Achievement Award etc. His other accolades include the Man of the Year Award (2002), Best Faculty Counselor Award (2022), and recognition as one of the Leading Engineers of the World (2007) etc. He has actively contributed to knowledge dissemination by attending over 50 conferences, workshops, seminars, training programs, and FDPs. As a guest lecturer, he has delivered impactful sessions at national and international events. Currently serving as Vice-President of QCT, Dr. Mehdi continues to inspire and shape the future of engineering education and research.

Sergey Suchkov[1-6*], Roger D. Kamm[9], Aleksandr Gabibov[11], Shawn Murphy[7,8], Arturo Solis Herrera[1], Holland Cheng[10]

[1]National Center for Human Photosynthesis, Aguascalientes, México

[2]Member, The Russian Academy of Natural Sciences, Moscow, Russia

[3]EPMA, Brussels, EU

[4]PMC, Washington, DC, USA

[5]ISPM, Tokyo, Japan

[6]AHA, Houston, TX, USA

[7]MGH, Boston, MA, USA

[8]Harvard Medical School, Boston, USA

[9]MIT, Cambridge, MA, USA

[10]T College of Biological Sciences, UC Davis, CA, USA

[11]Institute for Bioorganic Chemistry, The Russian Academy of Sciences, Moscow, Russia

Antibody-proteases as a generation of unique biomarkers, biocatalysts, potential targets and translational tools towards nanodesign-driven biochemical engineering and precision medical practice

The identification, impact and implementation of diagnostic, predictive and prognostic biomarkers of the next step generation becomes the Holy Grail of platforms, algorithms and protocols, which are the crucial for ***Personalized & Precision Medicine (PPM).*** High impact of Ab-proteases can be used to monitor both clinical and subclinical courses of chronic autoimmune inflammation to predict stepwise transformations of the course, starting from the pre-illness and to prognosticate the clinical illness finally. This information can allow to design the algorithms for combinatorial (preventive, prophylactic, therapeutic and rehabilitative) treatment, whilst developing unique tools for individually therapy for a number of diseases, such as a group of autoimmune diseases which holds a particular position.

Abs endowed with enzymatic properties have been isolated from the serum of patients with different autoimmune conditions. Disease-associated abzymes may have been "induced" by the Ag implicated in the disease and might precisely control a wide variety of physiological processes and thus are important drug targets. Regarding abzymes, their phenomenal property mentioned is buried in the Fab-fragment of the Ig molecule and is appearing to sound as a functional (Ag-binding and enzymatic) property of the Ab molecule.

The primary translational potential of abzymes (Ab-proteases, predominantly) and thus of this knowledge is in the rational design of new therapeutics to exploit the role of the key pathways in influencing disease. The latter is a brand-new field of chemical engineering. For instance, abzymes can selectively cleave the peptide bonds of the virus coat protein, thereby preventing the virus from binding to target cells.

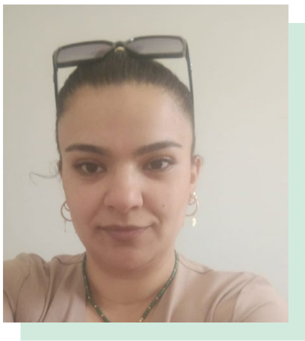
Of tremendous value are Ab-proteases directly affecting remodeling of tissues. By changing sequence specificity one may reach reduction of a density of the negative proteolytic effects within the myelin sheath and thus minimizing scales of demyelination.

Selective chemical modification of abzymes can be used to create novel proteins, particularly enzymes and Abs, with altered specificities and catalytic activities. Abzymes can be chemically engineered to make proteins of higher affinity or smaller molecular variants that retain or change the functional properties of the original Ab. In this context, targeted Ab-mediated proteolysis could thus be applied to isolate from Ig molecules catalytic domains containing segments to exert proteolytic activity and then be used as therapeutic modifiers. Ab-based therapeutics have entered the central stage of drug discovery as a result of a major shift in focus of many biotech and biopharma companies. Modification strategies should soon yield a wide spectrum of novel biomolecules whose activities are optimized for therapeutic applications.

Ab-proteases can be programmed and reprogrammed to suit the needs of the body metabolism or be designed for the development of principally new catalysts with no natural counterparts. Thus, abzyme study has an important value in theory and practice for biology, chemistry and medicine. So, further studies on targeted Ab-mediated proteolysis may provide biomarkers of new generations and thus a supplementary tool for assessing the disease progression and predicting disability of the patients and persons-at-risks. And the new approach is needed to secure artificial or edited Ab-proteases as unique translational probes to diagnose, to monitor, to control and to treat and rehabilitate autoimmune conditions patients at clinical stages and to prevent the disorder at subclinical stages in persons-at-risks to secure the efficacy of preventive, prophylactic and restorative manipulations.

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: National Center for Human Photosynthesis, Aguascalientes, México. The Russian Academy of Natural Sciences, Moscow, Russia. Member, New York Academy of Sciences, USA. 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.

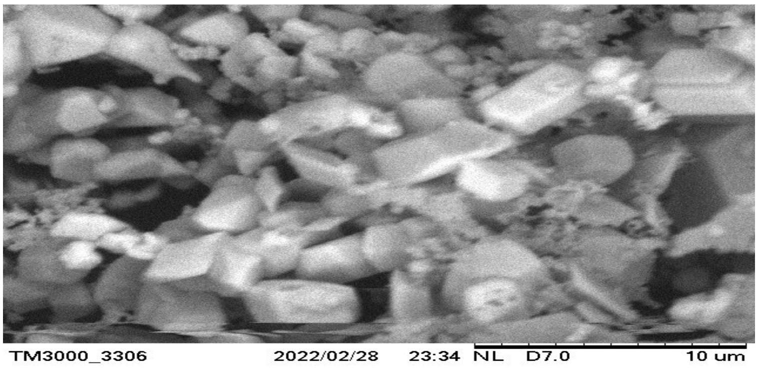


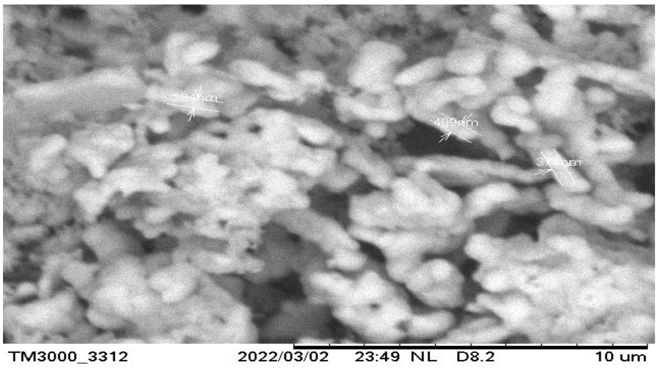
Sevda Hasan Aliyeva

İnstitute of Natural Resources of the Ninistry of science and Education of Republic of Azerbaijan, Nakhchivan State University, research worker

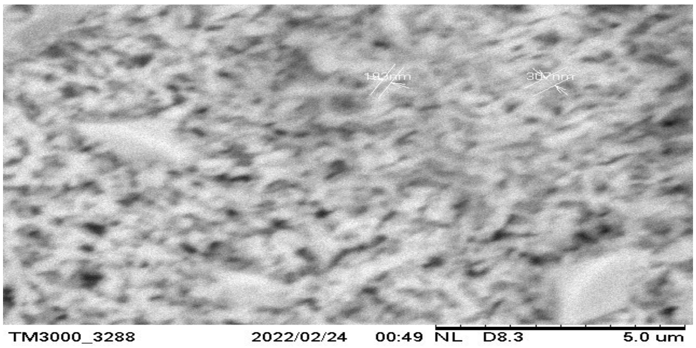
Microscopy of thallium thiostibate in some organic solvents

In this work, Tl3SbS4-nanocrystals were synthesized by solvotermal method in various organic solvents (ethylene glycol+polyetylene glycol). Optimal conditions for obtaining nanoparticles were determined (molar rations of the amount of components, volume ratio of the solvent, temperature, time, etc.) The crystal structere, morphology, nano-size and the obtained thallium thiostibitate nanocompound were studied usung a scanning electron mocricsope (SEM). During the experinments, potassium antimonyl tartrate was used as the antimony material, and a solution of sulfur in ethylenediamine was used as the sulfide material. The synthesis of Tl3SbS4 nanoparticles was carried out by adjusting the moolare ratio of sulfur to thalliuym and controlling the volume ratios of the solvent and the organic medium (ethylene glycol+polyetylene glycol and polyvinylpyrrolidonne). The process was carried out at a tempereature of 383-393K for 12 hours, and thallium-thiostibate nanoparticles were synthesized with a yiled of 89%. The results of scanning electron microscopy analysis showed that the synthesized thalkliuym thiostibitate nanoparticles had various shapes (wine-line, oval, quadrangular, triangular, etc.) and their sizes ranged from 180 to 400nm. The size of Tl3SbS4 nanoparticles obtained in ethylene glycol+polyethylene glycol medium was 250-700 nm, the size Tl3SbS4 nanopartciles obtained in polyvinylpyrrolidone medium was180-350nm. At the same time, a dispersed solution of thalliuym thiostibitate (Tl3SbS4) nanoparticles in n-heptane was prepared.





SEM of Tl_3SbS_4 nanoparticles prepared in ethylene glycol+polyethylene glycol medium



Morphology of Tl_3SbS_4 nanoparticles obtained in polyvinypyrrolidonr medium

Biography

Sevda Hasan Aliyeva, is graduated with nonors from the Azerbaijan State Oil Academy in 2008-2012 with a bachelor's degree in "Oil and gas and alternative energy texnology". She has graduated from the Azerbaijan State Oil Academy in 2012-214 with a master's degree in "Inorganic substances production technology". Since 2018, she has started ny her scientific actifity at the Nakhchivan branch of the Azerbaijan National Academy of Science. In 2019-2023, she was a doctoral candidate at the Nakhchivan branch of the Azerbaijan National Academy of Sciences and in 2025 she defended her scientific thesis on the topic "Obtaining thiostibitates from the interaction of antimony (V) sulfide with Ag1+, Cu1+, Cu2+, Tl1+ and Sb3+ ions in water and organic media and stydying their physicochemical". Currently, she is a research associate at the "Laboratory of Chemistry and Technology of Mineral Raw Materials" of the Institute of Natural Resources of the Ministry of science and education of the republic of Azerbaijan. She is also a teacher at Nakhchivan State universitity. She is the author of more than 25 scientific works.

Shawn Gouws*, Jason Mackay

Department of Chemistry, Nelson Mandela University, Gqeberha, South Africa

Characterization of OER catalysts for green hydrogen production via PEM water electrolysis

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 electrolyzers 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 utilizing PGMs such as iridium and platinum—as well as acid corrosion components.

Our research shows that similar robustness could be obtained for iridium only as the oxygen evolution reaction catalysts for the preliminary results for IrM (M=Ru, Ti, and Au) bimetallic mixtures. This paper will discuss the preliminary results through material characterization 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 electrolyzers 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.

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. Then joined the late Prof Ben Zeelie's group at InnoVenton, Nelson Mandela University, researching process chemistry and electrocatalysts. Has been published 15 articles in SCI journals, filled four patent applications, and written one book chapter. Dr. Shawn research interest is electrocatalysis for PEM water electrolysers to produce green hydrogen.

Stanislav Alexandra Alina

Department of Biochemistry, Medical Analysis Laboratory, Giurgiu County Emergency Hospital, Giurgiu, Romania

Testing the association between the UCP2 gene rs659366 with metabolic syndrome in patients with obesity from County Emergency Hospital Giurgiu Romania

Introduction: UCP2 is a protein that in humans is encoded by the UCP2 gene. The UCP2 gene is located genomically at 11q13.4 and plays a role in thermogenesis, obesity, diabetes mellitus and atherosclerosis. UCP2 has been associated with an increased risk of obesity in middle-aged individuals, and genetic variation in the UCP2 gene located at locus 4, defines the BMI polymorphism of the UCP2 gene, G/A (rs659366). The G/G and G/A genotypes have been associated with obesity. The -866G/G genotype has been associated with an increased risk of T2DM. UCP2 is a candidate gene for the development of DMT2. UCP2 plays a role in the metabolic syndrome, by downregulating insulin secretion and in the development of DMT2. The aim of the study is to test the association between the UCP2 rs659366 gene with MS in patients with obesity based on clinical data, laboratory investigations and genetic methods.

Material and Method: The study was conducted on 75 subjects from the Giurgiu County Emergency Hospital, 55 with Obesity (OB) and 20 controls, based on clinical data: BMI, HTA, sex and age, biochemical laboratory investigations: Glucose, triglycerides, cholesterol, HDL, LDL, uric acid, magnesium, Hba1c performed on the BS300 device and hematological BS3000 mindray for HLG: WBC, RBC, HGB, and HCT. The polymorphisms of the UCP2 rs659366 gene were sequenced by the RFLP-PCR method and the Advenced NGx test. The results were processed by the Graph Pad Prism 7.0.3, MDR 3.0.2 and Matlab R2009b programs.

Results: It results that the UCP2 rs659366 polymorphisms have predominantly 20 homozygous and 9 heterozygous genotypes that showed increased values of glucose concentrations and HbA1c are associated with cardiovascular diseases, diabetes and obesity, which may increase the risk of MS. It results that the UCP2 gene with UCP2 rs659366 (OR>1 and p<0.0001, OR=2), presents an increased risk of developing MS.

Conclusions: The UCP2 gene is associated with metabolic syndrome.

Biography

Stanislav Alexandra Alina is a medical biologist specialist at the Department of Biochemistry within the Medical Analysis Laboratory of the Emergency County Hospital Giurgiu Romania and completed PhD at the age of 35 at the Department of Genetics, Faculty of Biology, University of Bucharest. Stanislav Alexandra have studies in classical and modern methods of human genetics, biochemical and hematological laboratory investigations, clinical aspects (Metabolic syndrome, obesity, diabetes mellitus and hypertension, risk factors and bioinformatics methods, epigenetics (Alzheimer's), microbiology (Staphylococcus aureus), Immunology, Biochemistry, Electrophoresis, Ionometry and HbA1c and Matlab programming, RFLP-PCR and Advanced NGx.

T.N. Chhowala

Department of Chemistry, Veer Narmad South Gujarat University, Surat, Gujarat, India

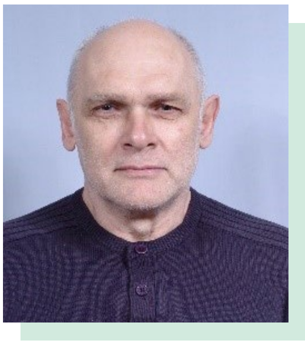
Remedial effects of chemotherapy and hyperthermia of complexes for breast cancer cells

Nano complexes are antibacterial, anticancer, anti-inflammatory, and antimicrobial capabilities, which have drawn particular attention as a potential class of medicinal medicines. Nano complexes [Nano-magnetite-Lys@Cu(PPh3)I] and [Nano-magnetite-Arg@Cu(PPh3)I] with sizes of 12 nm and 15 nm are reported to have undergone a multi-step synthesis and characterization process. Complexes significantly outperformed the conventional medicine cis-platin. Remedial combined effects of hyperthermia and chemotherapy can make both complexes a double-edged sword in the treatment of breast cancer. Additionally, they have minimal toxicity, are inexpensive, and quickly undergo redox reactions, which enable a range of ligands to combine to produce stable and biologically effective complexes.

Keywords: Hyperthermia, chemotherapy, breast cancer, inexpensive

Biography

Dr. Tarulata N Chhowala studied Chemistry at the Veer Narmad South Gujarat University, Surat and graduated as M.Sc in 1999. She then joined the research group of Prof. K.R.Desai and served as Assistant Professor since 2007 and also received her PhD degree in 2009 at the same institution. She also obtained the position of an Associate Professor in 2022. She has published more than 14 research articles in reputed journals.



Valery P. Kalinitchenko[1,2*], Valery P. Meshalkin[3], Mikhail G. Baryshev[2], Mikhail A. Sevostyanov[2], Sergey V. Gudkov[4], Tatiana M. Minkina[5], Saglara S. Mandzhieva[5], Svetlana N. Sushkova[5], Vishnu D. Rajput[5], Dmitry A. Makarenkov[6], Vladimir V. Chernenko[1], Georgiy S. Larin[1]

[1]Institute of Fertility of Soils of South Russia, Persianovka, Russia

[2]All-Russian Phytopathology Research Institute, Big Vyazyomy, Russia

[3]D. Mendeleev University of Chemical Technology of Russia, Moscow, Russia

[4]Prokhorov General Physics Institute of the Russian Academy of Sciences, 119991, Vavilova St., 38, Moscow, Russia

[5]Southern Federal University, Rostov-on-Don, Russia

[6]Institute of Chemical Reagents and High Purity Chemical Substances of National Research Centre "Kurchatov Institute", Moscow, Russia

Chemical-soil-biological engineering and biogeosystem technique methodology in shaping sustainable future

Current "Ecosphere–technology" conflict stems from a chemical, environmental and agricultural management outdated technological platform. The platform basis is a simplified attempt in imitating natural phenomena in technology. A standard chemical-technological system hierarchy defines a priority level its own technological waste disposal as low, and waste becomes an ecosphere chemical-technological load. Poor soil geophysical system and fertility under the uncontrolled chemical waste deposition reduces the soil productivity and ecosphere health and sustainability.

A critical reassessing of the land and water use, waste recycling technologies, environment and agronomy practice is needed to eliminate shortcomings and configure a future sustainable environmentally sound chemical-soil-biological engineering.

Using a heuristic approach to understand an origin of an environmentally sound technological development niche, we developed the Chemical-Soil-Biological Engineering (CSBE) methodology and Biogeosystem Technique (BGT*) methodology.

The CSBE-BGT* objects are: main product chemical-technological system; devices for improving the geophysical and geochemical properties of soil by synthesizing the structure and architecture of its illuvial layer for the biological-soil recycling of bulk or granular by-product; pulsed intra-soil sequential-discrete devices for recycling of liquid by-product and/or soil moistening and plant nutrition; and an environmentally friendly biological production.

CSBE-BGT* is capable in providing: a main chemical product full-waste-free technology; a dispersed by-products recycling within the synthesized fine-aggregate architecture of the soil inner layer for a plants favorable development; and a food, fodder and row material economic use of the biological production obtained on the synthesized soil.

BGT* applies nature phenomena creating a nature-friendly technical means and technologies for a long-term soil geophysical, chemical, water and biological properties optimization. The BGT* based one time 20–50 cm layer intra-soil milling provides a stable soil fine multilevel aggregate system improving a soil biome function for up to 40 years. The BGT* based intra-soil pulse continuous-discrete watering reduces a plant water consumption circa 5–20 times compared to the standard irrigation. BGT* based municipal, industrial waste and gasification byproduct intra-soil dispersed recycling in a course of 20–50 cm soil layer milling provides soil solution equilibria control, heavy metals passivation, environmental safety and plant nutrition. Using BGT* methodology, the yield becomes higher for 50–80% compared to standard technology. BGT* methodology promotes the soil system continuity, reinforces soil biogeochemical turnover, ensures reversible carbon intra-soil and aboveground biological sequestration, biosphere health and climate system sustainability.

There is a strong need to use a CSBE-BGT* in chemical-biological engineering theory and practice. The CSBE-BGT* helps in understanding the new world chemical engineering development niche. The CSBE -BGT* expands the environment, soil science, agronomy, irrigation, waste recycling fields as well as the corresponding new technical equipment design and manufacturing. The CSBE-BGT* provides a practical solution to a friendly environment synthesis and make a designer’s job more efficient focusing on the new high level developments improving the accuracy of a design. The CSBE-BGT* methodology provides new information to assist in a design problem.

CSBE-BGT* is a circular green chemistry waste free environment friendly and biosphere high quality, productivity and health platform shaping a sustainable future.

Biography

Professor Dr. Sc (Biol) Valery P. Kalinitchenko. Candidate of Science Degree from Moscow State University, in 1984. Doctoral of Science Degree from Moscow State University, in 1991. Don State Agrarian University, Agriculture and Land Reclamation Department Chair, Persianovka, Russia, in 1976-2012. Institute of Fertility of Soils of South Russia Persianovka, director, from 2003 till now, and All-Russian Phytopathology Research Institute, Big Vyazemy, Russia, leading researcher from 2016 till now. Research interests: Soil and water saving, waste recycling, biosphere sustainability, soil high productivity and health, soil chemical equilibria, Chemical-Soil-Biological Engineering and Biogeosystem Technique. Author: 700 monographs, journal and conference papers and 50 patents. Editor-in-Chief: Biogeosystem Technique.

Chaoji Xiong[1], Bin Wu[1], Kun Liang[1], Chunhua Wu[1], Xiaoping Rao[2], Wei Wu[3*], Qian Chen[1]

[1]Key Laboratory of State Forestry and Grassland Administration on Highly-Efficient Utilization of Forestry Biomass Resources in Southwest China, College of Materials and Chemical Engineering, Southwest Forestry University, Kunming 650224, China

[2]Academy of Advanced Carbon Conversion Technology, Huaqiao University, Xiamen 361021, China

[3]Department of Physics and London Centre for Nanotechnology, University College London, London, United Kingdom

The powerful capacities of polymers for the adsorption of the mercury ions in water

Mercury ions (Hg^{2+}) are among the most hazardous pollutants in wastewater, posing serious threats to environmental sustainability and human health. However, many current adsorbent materials suffer from limited adsorption capacity and rely on costly raw materials. There is, therefore, an urgent need for low-cost adsorbents with high efficiency.

Our team has recently integrated advanced chemical synthesis techniques, comprehensive material characterization, and first-principles calculations based on density functional theory to explore polymeric and network-based materials for Hg^{2+}removal. Our adsorbents have demonstrated exceptional performance, with removal capacities reaching up to 2562 mg g^{-1}.

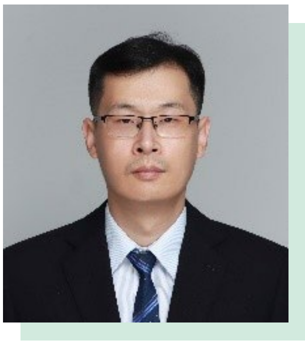
We have investigated a thiophene-based porous triazine polyamide, whose unique molecular architecture exhibits strong affinity toward mercury ions. Additionally, a thiophene-network polyamide incorporating tri(4-aminophenyl)benzene functions like a precision-woven "molecular filter," effectively capturing mercury ions. A porous polyamide based on 2,5-furandicarboxylic acid offers abundant internal surface area—providing more "habitats" for ion adsorptions. Morever, we have researched on the thio-group-modified covalent triazine polyamide, which, after clever modification, has a significant leap in the capture of mercury ions. The triazine-based sulfur-containing polyamide, the introduction of sulfur element is like a powerful "adsorption engine" for it.

Beyond these, we have explored several novel polymeric materials that show strong potential for mercury ion removal from water. These emerging materials offer a promising new direction for water purification technologies, highlighting a path toward the development of environmentally friendly and highly effective mercury adsorbents.

We thus envision a bright future for these materials in wastewater treatment, contributing to cleaner water and a more sustainable environment.

Biography

Dr. Wu earned Ph.D. in Physics from University College London. Following doctoral studies, conducted research at both University College London and Imperial College London. Has been published over 60 papers in peer-reviewed journals including Nature Communications, Advanced Materials, ACS Nano and NPG Asia Materials. Dr. Wu also supervised more than 20 MSc students across various topics in theoretical physics and materials modelling, as well as co-supervised Ph.D. students. Dr. Wu also serves as a referee for leading journals, including npj Quantum Materials, Advanced Functional Materials, Advanced Optical Materials, Journal of Chemical Engineering, and JACS.



Xun Yuan

School of Materials Science and Engineering, Qingdao University of Science and Technology, Qingdao 266042, PR China

Surface engineering of ultrasmall metal nanoclusters for biomedical applications

Metal Nanoclusters (MNCs) have attracted considerable attention in the fields of catalysis and biomedicine due to their ultrasmall size, unique molecular-like properties, rich surface chemistry, good biocompatibility and stability. This report will introduce the progress in the synthesis and application of MNCs from the following aspects: 1) To address the challenges of size control and unclear growth mechanism of MNCs, a universal synthesis method was designed to regulate the reduction kinetics of the reducing agent, achieving controllable tuning of the size of MNCs and revealing the growth mechanism of MNCs of different sizes. 2) By surface engineering, two types of Pt NCs-based catalysts were developed for Hydrogen Oxidation Reaction (HOR) in alkaline media. Theoretical simulations revealed the decisive role of the surface chemistry of Pt NCs in regulating the adsorption and desorption of *H/*OH/CO and the generation of H_2O, endowing them with superior catalytic activity and high stability compared to Pt single atoms and Pt particles. Additionally, this catalyst can exhibit high tolerance to CO by weakening the binding energy of CO intermediates. 3) By modifying the surface of Au NCs with different functional molecules, a series of MNC-based theranostic probes were constructed to achieve NIR-II luminescence imaging guided disease treatment. These works may deepen the understanding of MNCs at the atomic level and promote their application in catalysis and biomedicine.

Biography

Dr. Xun Yuan received Ph.D. degree (2014) from National University of Singapore under the supervision of Prof. Jianping Xie. After 3 years of postdoctoral work at the Institute of Bioengineering and Nanotechnology (IBN, Singapore), then joined Qingdao University of Science and Technology (QUST) as a professor in 2017. Dr. Xun research focuses on the synthesis and applications of metal nanoclusters. Has been published more than 100 research articles in SCI (E) journals with total citations of more than 10000 times.

Zerihun Assefa

Chemistry Department, North Carolina A&T State University, USA

Modulation of structural and spectroscopic properties in a series of metal atoms ranging from transition to lanthanide to actinide atoms connected through bridging ligands

The structural features and spectroscopic properties of metal atoms connected through bridging ligands is fascinating. The metal atoms covered in this talk range from transition metals to lanthanides and some of the heaviest actinide metals in the periodic table. Our lab has been attempting for several years to linking more than two metal atoms through bridging ligands. Low dimensional structural motifs are dominant in these complexes. The metal–metal interactions between adjacent metal atoms provide highly tunable spectral properties that can be tuned by chemical and physical variations such as choice of counter cation, temperature or, applied pressure. In this presentation correlation between the structural motifs and emission behavior will be discussed for several complexes containing late transition metals and lanthanide and/or actinide metals. Both the structural features and the spectroscopic properties are dominated by the presence of ground and excited state metal-metal interactions as the result of the common low dimensional motifs. The spectroscopic part of this talk will cover some of the unique phenomenon exhibited by these complexes including multiple state emissions, energy transfer, and dual donor emission enhancement. Some unusual luminescence behaviors, such as exciplex and excimer emissions resulting from the unique structural motifs are also discussed on a variety of late transition metal based coordination polymeric compounds.

Biography

Dr. Assefa obtained BSc degree from Addis Ababa University and PhD in 1992 from the University of Maine, served as a post-doctoral fellow at Texas A&M, and Auburn University focusing in the areas of X-ray crystallography and multi- electron transfer kinetics, respectively. In 1995, Dr. Assefa joined the Oak Ridge National Laboratory and primarily conducted basic research on transuranium elements. Then moved to North Carolina A&T State university to pursue academic career. Dr. Assefa has pursued fundamental research on materials for luminescent sensor application, white light emitting materials, and gold and other Group 11 metal compounds for medicinal applications. Has been published over eighty-five peer-reviewed articles and three book chapters.

Dr.Yogita Shinde*, Zohra Ulfat Shaikh*

Department of Chemistry, KC College Churchgate Mumbai
20, HSNC University, Mumbai, India

Monitoring heavy metal pollution in Bandra lake with EDX: A study of seasonal variation at 30 days interval

The purpose of this project is to use Energy-Dispersive X-Ray Analysis (EDX) to detect and track heavy metals in Bandra Lake (Mumbai, Maharashtra, India) water samples. To improve the identification of trace metals, a preconcentration procedure is used in conjunction with thecollection of water samples from reliable sources. EDX is appropriate for environmental monitoring because it provides quick, multi-element analysis without causing sample damage. With an emphasis on components like iron, copper, zinc, and lead, the study evaluates the temporal fluctuations in heavy metal concentrations. This study contributes to environmental conservation efforts by using EDX to give insights on Bandra Lake's water quality over time. Understanding the dynamics of heavy metal contamination and developing mitigation methods for its effects on aquatic ecosystems will be made easier by the findings.

Keywords: Heavy Metals, Energy-Dispersive X-Ray Analysis (EDX), Water Quality Monitoring, Seasonal Variations.

Biography of Yogita Shinde

Dr Yogita Shinde born on April 22 1973 is a renowned academician and an analytical chemist. With over 20 years of teaching experience in Undergraduate and post graduate Chemistry she has been instrumental in training students in the subject of analytical chemistry. She has a special liking for environmental chemistry and food and cosmetic chemistry. She has been an active organiser of several intercollegiate and intracollegiate events. She has been a coordinator for pg courses at KC College. During her affiliation to University of Mumbai she has served as a chairperson for MSc analytical chemistry. Catering to almost 500 students across the university. She has to her credit several papers published in peer reviewed journals.

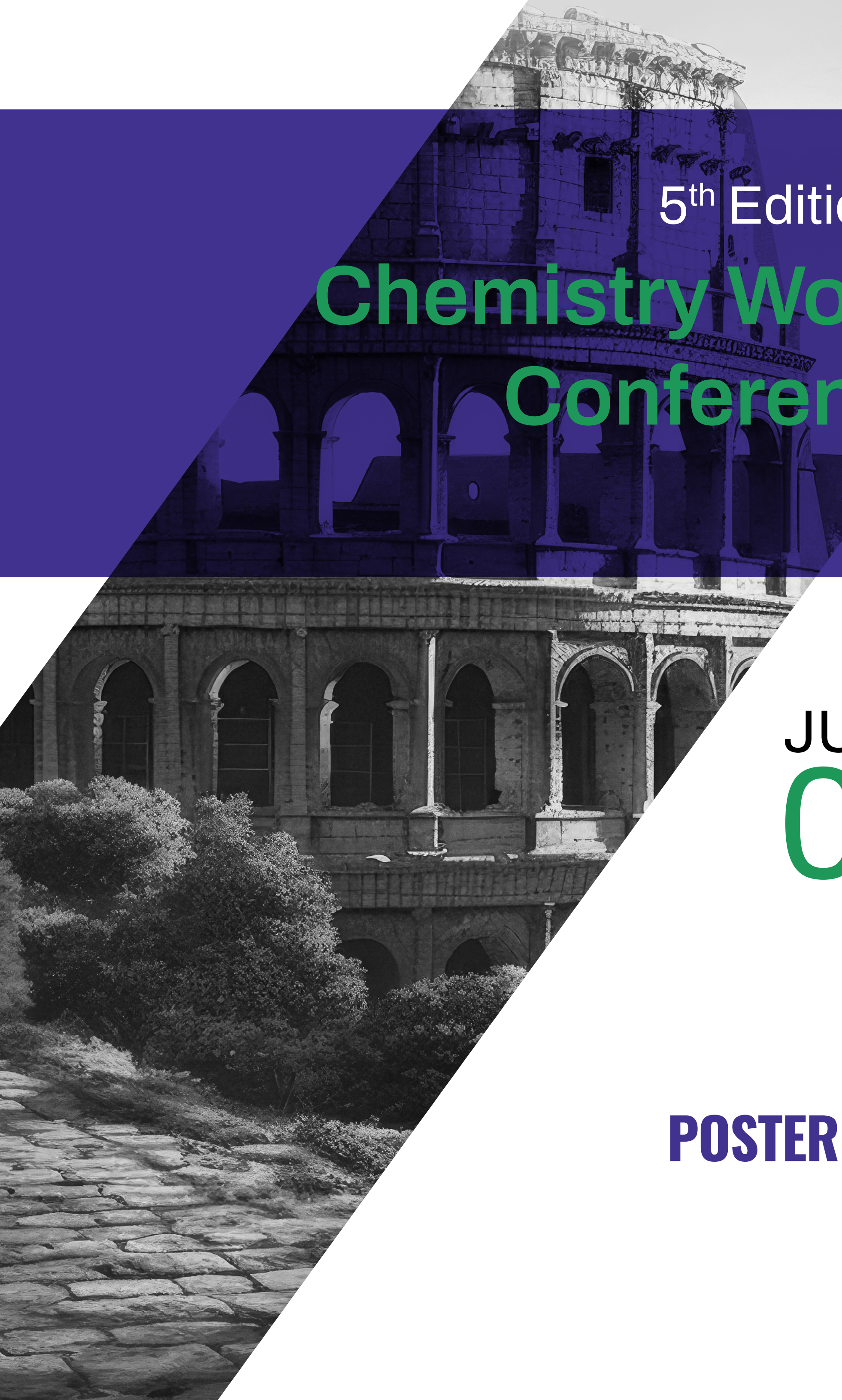
Biography of Zohra Ulfat Shaikh

Zohra Ulfat Shaikh, born on March 23, 1992, in Mumbai, India, is an accomplished academic and chemistry lecturer with a strong foundation in analytical chemistry. She earned her B.Sc. and M.Sc. degrees in Chemistry from Mumbai University, achieving commendable results, and is currently pursuing her Ph.D. at HSNC University. With over seven years of teaching experience at RD & SH National College and Mithibai College, she has significantly contributed to academia by mentoring students and serving as an examiner and moderator for various practical examinations under Mumbai University.

Zohra's leadership skills were evident when she chaired the Chemistry Festival (Fluorescence) in 2016 at R.D. National College, earning recognition for her organizational abilities. She has also conducted workshops on dyeing fabrics for students, showcasing her commitment to practical education. Fluent in Hindi, Urdu, and English, Zohra is adept at public speaking and dramatics, which complement her teaching expertise.

Beyond academics, she enjoys creative pursuits such as soap making, tie-dyeing, and fabric painting, alongside physical activities like yoga and badminton. Her dedication to education and multifaceted interests make her a dynamic individual committed to personal growth and contributing to the field of chemistry.

BOOK OF ABSTRACTS



5th Edition of

Chemistry World Conference

JUNE
02-04
2025

POSTER PRESENTATIONS

Daniel Makanyane[1], Lindokuhle Mabuza[2], Phikelelani Ngubane[2], Andile Khathi[2], Allen Mambanda[1] and Irvin Noel Booysen[1]*

[1]School of Chemistry and Physics, University of KwaZulu-Natal, Pietermaritzburg, South Africa

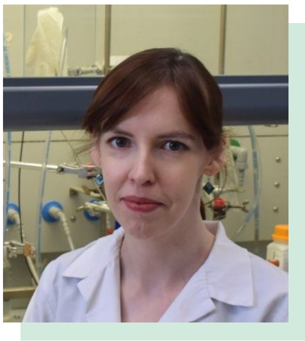
[2]School of Laboratory Medicine and Medical Sciences, University of KwaZulu-Natal, Pietermaritzburg, South Africa

Anti-amyloid aggregation and anti-hyperglycemic activities of ruthenium uracil Schiff base compounds and their chitosan-polyvinyl alcohol electrospun nanofiber conjugates

Our earlier studies on a leading uracil-Schiff base chelated ruthenium compound, [Ru(H3ucp)Cl(PPh3)] (1) (H4ucp = 2,6-bis-((6-amino-1,3-dimethyluracilimino)methylene)pyridine) showed it can serve as a candidate metal-based drug in an anti-diabetic animal model.[1] Most recently, we have illustrated that the structural features of 1 and its derivatives dictate their mechanism of anti-diabetic action.[2] Solution chemical reactivities of the different ruthenium complexes were rationalized by density functional theory computations. Furthermore, the binding affinities and strengths between BSA and the respective ruthenium complexes were monitored using fluorescence spectroscopy. The diimine bis-uracil metal complexes could disintegrate mature amylin amyloid fibrils, while the mono-imine uracil metal complexes showed comparable disaggregation capabilities for the BSA (ThT) amyloidal plaques. In addition, the in vitro anti-diabetic activities of the novel metal complexes were assessed in selected skeletal muscle and liver cell lines. In the pursuit to develop proficient metallopharmaceuticals for Diabetes Mellitus (DM), the lead metal complex and its analogs were individually incorporated into nano-confined polymer frameworks to investigate their corresponding drug-release profiles and glucose-lowering effects in selected cell lines in a time-dependent manner. In particular, chitosan (CS)-polyvinyl alcohol (PVA) electrospun nanofibers (CS-PVA ENFs) containing the different ruthenium uracilimino complexes (Ru) were fabricated by in situ electrospinning. The resultant guest-host nanoconjugates were characterized by Scanning Electron Microscopy - Energy Dispersive X-ray (SEM-EDX), powder X-ray diffraction, and FTIR spectroscopy.

Biography

Prof Irvin Noel Booysen graduated in 2010 with a PhD in Inorganic Chemistry from Nelson Mandela University. Subsequently, he was hosted as a postdoctoral fellow at the Nanotechnology Innovation Centre of Rhodes University. He is an Associate Professor in Inorganic Chemistry at the University of KwaZulu-Natal. Prof Booysen's research focuses on Bio-inorganic chemistry and electrochemical sensor development. In addition, he has been awarded several competitive research grants, such as the Republic of South Africa Medical Research Council, the Jamaica-RSA Bilateral, and Nuclear Technologies in Medicine and the Biosciences Initiative (NTeMBI) research grants.



Jekaterina Ivanova[1*], Raivis Žalubovskis[1,2]

[1]Latvian Institute of Organic Synthesis, 21 Aizkraukles St., LV-1006, Riga, Latvia

[2]Institute of Technology of Organic Chemistry, Riga Technical University, 3/7 Paula Valdena St., LV-1048, Riga, Latvia

Synthesis and biological evaluation of novel TrxR inhibitors as anti-cancer agents

Cancer is a major public health problem and a leading cause of death worldwide, accounting for nearly 10 million deaths in 2020, or nearly one in six deaths.

In spite of the existence of several approaches for the treatment of cancer it is still a challenge for the scientific community. High mortality level among cancer patients clearly points out low efficiency of chemotherapeutical drugs currently used in clinics and the desperate need to develop new and effective anti-cancer drugs with novel mechanism of action.

Elevated reactive oxygen species and antioxidant defense systems have been recognized as one of the hallmarks of cancer cells. As a major regulator of the cellular redox homeostasis, the selenoprotein thioredoxin reductase (TrxR, EC 1.8.1.9) is increasingly considered as a promising target for anticancer drug development. 2,3 Inhibiting thioredoxin reductase (TrxR) to disrupt the redox equilibrium and induce tumor cell apoptosis is a significant tumor therapeutic strategy.

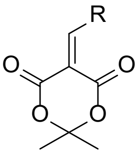
Thioredoxin reductases (TrxRs) are NADPH-dependent flavoenzymes–the only known enzymes that reduce thioredoxin (Trx) from its oxidized form (Trx-S_2) to reduced one (Trx-$(SH)_2$).

TrxR1 is highly expressed in many cancer cells, therefore it is a promising target for the development of novel anticancer agents.

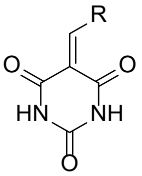
Considering all mentioned above this project is devoted to the development of novel anti-cancer agents – TrxR inhibitors. The aim of this research is to obtain a series of potential TrxR derivatives and determine their biological activity.

As Michael acceptors are well known TrxR inhibitors, we decided to check if cyclic derivatives with Michael acceptor moiety as well as one more carbonyl group may serve as TrxR inhibitors.

Here we present the series of derivatives of Meldrum's acid 1 and Barbituric acid 2 as potential TrxR inhibitors (Picture 1).



1



2

Picture 1. Derivatives of Meldrum's acid and Barbituric acid.

Biological screening of all the synthesized compounds was performed (in vitro enzymatic on TrxR1).

Acknowledgement: This research is supported by RRF grant No.49/OSI/PG (RRF project No.5.2.1.1.i.0/2/24/I/CFLA/001).

Biography

Dr. chem. Jekaterina Ivanova studied Chemical Engineering at Riga Technical University, Latvia, and graduated as MS in 2012. Since 2007, has been working at Latvian Institute of Organic Synthesis under the supervision of prof. Raivis Žalubovskis. She received her PhD degree in Medicinal Chemistry from Riga Technical University in 2018. Dr. Jekaterina is a co-author of two patents and 18 research articles. In 2017 she received L`ORÉAL Baltic "For Women In Science" fellowship with the support of the Latvian National Commission for UNESCO and the Latvian Academy of Sciences. Also received Achievement in Science Award 2023 from the Latvian Academy of Sciences.

Justin Jian Qiang Mah[1,2*], Hongzhi Feng[3], Nayli Erdeanna Binte Surat'man[3], Bofan Li3, Sheng Wang[3], Zibiao Li1,[3,4]

[1]Institute of Materials Research and Engineering (IMRE), A*STAR, Singapore

[2]Division of Chemistry and Biological Chemistry, Nanyang Technological University, Singapore

[3]Institute of Sustainability for Chemicals, Energy and Environment (ISCE2), A*STAR, Singapore

[4]Department of Materials Science and Engineering, National University of Singapore, Singapore

Water-resistant boronic ester vitrimers via hydrophobic side chain protection

To address the limitations of boronic ester-based dynamic polymers in moist or aqueous environments, we developed a boronic ester vitrimer system enhanced with hydrophobic fluorinated side chains. These materials are capable of withstanding high humidity and even direct water immersion without degradation in thermal or mechanical performance. The vitrimer, termed FV1, was synthesized via radical copolymerization of a fluorinated acrylate monomer and a diol-functional acrylate, followed by dynamic crosslinking using 1,4-phenylenebisboronic acid.

Characterization confirmed the successful incorporation of functional groups and formation of a stable network. FV1 retained its properties under 65% RH for 7 days and showed negligible mechanical degradation after 1 hour of water immersion. Comparative studies with a non-fluorinated analogue revealed significant performance gaps, highlighting the efficacy of hydrophobic shielding over the boronic ester linkages. Furthermore, FV1 demonstrated robust self-healing and could be both mechanically and chemically recycled under mild conditions using green solvents, such as methanol.

These findings present a significant step toward the practical use of dynamic covalent materials in humid or aqueous environments, advancing the design of circular polymers with durability and recyclability in real-world conditions.

Biography

Justin Mah is a PhD student at Nanyang Technological University, currently attached to the Institute of Materials Research and Engineering (IMRE), A*STAR. His research focuses on sustainable polymer materials with dynamic covalent chemistries, particularly in enhancing durability and recyclability.

Karolina Olechowska[*]**, Beata Wyżga, Katarzyna Hąc-Wydro**

Department of Environmental Chemistry, Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland

Membrane activity of honokiol, an antimicrobial agent for enhanced safety and sustainability – studies in model systems

Antimicrobial resistance has developed as one of the major urgent threats to public health. Due to clinical and epidemiologic significance of this issue, there is an increasing demand to search for innovative and safe antimicrobial substances for healthcare, agriculture, food and cosmetics production. A very promising approach in this matter is the use of substances of natural origin, that exhibit wide range of biological properties. Honokiol, a polyphenolic compound, present in bark extract of Magnolia officinalis, shows the potential to work as an antibacterial, anti-inflammatory, anticancer, antioxidant and neurotherapeutic agent. However, despite many studies on the effect of this substance on bacterial cells, its molecular mechanism of action still requires verification. It is assumed that the first site of honokiol action against bacterial cells is cell membrane and the structure of membrane lipids may have the significant influence on honokiol antibacterial activity. Therefore, the aim of the presented research was to analyze the effect of honokiol on the properties of model bacterial cell membranes, considering differences in lipids structure. The investigations were performed for membrane-mimicking systems formed from individual lipids characteristic for bacterial membranes (phosphatidylethanolamines, phosphatidylglycerols and cardiolipins) and from multicomponent mixtures of this lipids (imitating Escherichia coli and Staphylococcus aureus membranes). The results of this experiments allowed to analyse the effect of the lipid structure, i.e. polar headgroup (POPE vs POPG comparison) and hydrophobic chain (TOCL vs TSCL comparison) on the interactions with honokiol. As model membranes Langmuir monolayers and liposomes were be applied. Based on experiments conducted using various techniques (Brewster angle microscopy, dynamic light scattering, fluorescence anisotropy) the influence of honokiol on intermolecular interactions, stability, organization and morphology of artificial cell membranes in the context of its membrane-related antibacterial properties were assessed.

Acknowledgments: This work has been supported by a grant from the Faculty of Chemistry under the Strategic Program Excellence Initiative at Jagiellonian University.

Biography

PhD Karolina Olechowska received her MSc degree in chemistry in 2015 and PhD degree in 2019 (with the distinction for doctoral dissertation), from the Faculty of Chemistry at the Jagiellonian University. Since 2018 employed at the Department of Environmental Chemistry at the same institution as a member of Physicochemical Environmental Research Group. Her scientific interests focus on cell membrane modeling, the search for antimicrobial agents of natural-origin, and the development of nanostructured drug delivery systems.

Mohammed Hussien[1*], Richard Barker[2], David Harbottle[1], Peter Wilkie[3], Timothy Hunter[1]

[1]School of Chemical and Process Engineering, University of Leeds, Leeds, United Kingdom

[2]School of Mechanical Engineering, University of Leeds, Leeds, United Kingdom

[3]Roemex Ltd, Aberdeen, United Kingdom

Evaluation of a novel corrosion inhibitor for lead sequestration in aqueous systems

This work presents a detailed investigation into the solution stability and lead-binding performance of a polymer-based corrosion inhibitor, through a collaborative project between Roemex Ltd and the University of Leeds. Thermogravimetric analysis (TGA) indicated that the inhibitor contained primary components of sodium polyaspartate polymer, and ADBAC surfactant. Stability testing confirmed the inhibitor remains stable at high concentrations (up to 500 ppm) and under acidic conditions (pH < 7), making it suitable for diverse application environments.

Turbidity and visual inspection tests demonstrated the polymer's ability to interact with lead ions (Pb^{2+}), with clear precipitation observed at elevated concentrations (200 ppm of $PbCl_2$ or $Pb(NO_3)_2$). Dynamic Light Scattering (DLS) measurements revealed the polymer forms large globules in solution, which shrink in the presence of 1% NaCl, confirming that ionic strength influences polymer conformation and solubility. Atomic Absorption Spectroscopy (AAS) using both membrane filtration and direct extraction methods showed that the polymer sequesters over 90–95% of Pb^{2+} ions at higher concentrations. Additionally, the inhibitor showed clear selectivity for lead ions over Ca2+, as an analogue for other divalent metals present in the environment, where polymer stability was maintained even in elevated levels of calcium. These findings confirm the inhibitor's potential to capture lead efficiently and highlight its possible applications in industrial corrosion control and environmental remediation.

Outside of the polymers interaction with dissolved lead, investigations were conducted into whether it acts to accelerate leaching from lead scale surfaces ($PbCO_3$ and PbS). Additional work also included electrochemical corrosion testing with polymer-coated lead surfaces, to understand how corrosion inhibition is influenced by background free lead ions in the solution.

Biography

Dr. Mohammed Hussien received his PhD in Mechanical Engineering from the University of Huddersfield in 2023, focusing on high entropy alloy protection in oil recovery. He previously earned an MSc in Oil & Gas Engineering with Management and has over 15 years of experience in the oil and gas industry, including a long tenure at Waha Oil Company. Dr. Hussien has also served as a teaching assistant and research fellow and is currently a Research Fellow in Multiphase Flows and Corrosion Science at the University of Leeds.

MS. Mona Nasar* (M.A), Dr. Elena Bekovetsky (Ph.D.)

Ziv Medical Center, Zefat, Isreal

Improving point-of-care testing accuracy through training and supervision

Point-of-Care Testing (POCT) involves conducting laboratory tests near the patient rather than in a central laboratory, offering faster Turnaround Times (TAT) and enabling immediate clinical decisions. However, POCT is often performed by non-laboratory personnel, increasing the risk of human errors that may impact diagnostic accuracy.

Several factors contribute to POCT errors, including incorrect patient identification, spontaneous patient number assignment, improper test procedures, and sample rejection. These errors can lead to misdiagnoses, delays in treatment, and compromised patient care. Addressing these challenges requires structured training, continuous monitoring, and systematic interventions.

This study evaluates the impact of POCT training programs, random observations, and the implementation of a personal identification code for medical staff on reducing common errors. The primary focus is on minimizing spontaneous patient number assignments and sample rejections, which are among the most frequently encountered issues in POCT.

Our results demonstrate that with consistent POCT manager supervision and intervention, there is a measurable reduction in both error types. Over time, the combination of structured training, real-time monitoring, and accountability measures significantly improves test accuracy and reliability. Additionally, the impact of interventions across most departments is reflected in the increase in calls to the POCT manager and the number of training sessions. However, the gradual decrease in these calls and training requests over time suggests that medical staff have become more competent, leading to improved result quality and overall efficiency.

In conclusion, effective training and systematic interventions play a crucial role in reducing POCT-related errors. Implementing a structured approach that includes continuous education, random audits, and staff accountability measures enhances test accuracy, improves diagnostic efficiency, and ultimately contributes to better patient outcomes.

Biography

Mona Nassar, is the POCT Department Manager at Ziv Hospital in Zefat, specializing in biochemistry, endocrinology, and laboratory management. With over ten years of experience in clinical diagnostics, established the hospital's POCT department in 2017, introducing more than 50 medical laboratory devices to enhance diagnostic services. Mona Nassar oversees their performance, ensuring monthly quality control and compliance with laboratory standards. As a member of the paramedical committee, she is dedicated to improving laboratory operations and advancing patient care. Mona is an actively collaborates with healthcare professionals to optimize diagnostic accuracy and efficiency. Through continuous research, innovation, and professional development, she strives to enhance laboratory science, implement cutting-edge technologies, and improve healthcare outcomes for better patient management.

Prayash Chakraborty

UG-Medical (MBBS) Course (II year) Jagannath Gupta Institute of Medical Sciences & Hospital Budge budge, Calcutta–700137, India

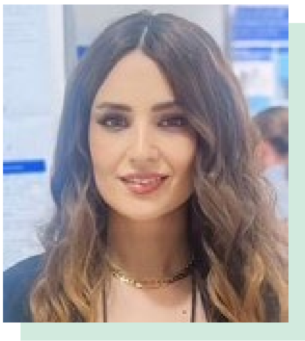
Interdisciplinary studies in pharmacology, pathology, microbiology and chemistry in undergraduate course of medicine: A real outcome based learning in mode of action of drugs and identification of diseases

Interdisciplinary research in pharmacology, pathology, microbiology and chemistry combines expertise in drug discovery, development and mode of action with chemical principles and techniques. This collaboration leads to a deeper understanding of how drugs interact with the body, ultimately improving drug design and therapeutic outcomes. By combining chemical knowledge with biological understanding, researchers can design more effective and targeted drugs. We have learnt that this kind of interdisciplinary research can optimize drug formulations, ensure drug stability and enhance drug delivery systems. This approach also allows for a more detailed examination of how drugs affect the body at the molecular level, leading to a deeper understanding of drug action and mechanisms of disease. The combined study, often called chemical microbiology, combines expertise from different disciplines like genetics, biochemistry and organic chemistry that enable us to analyze the behavior of microorganisms. This lucrative area of research combines expertise from different disciplines like genetics, biochemistry and organic chemistry to analyze the clinical biochemistry, chemical pathology and behavior of microorganisms. This combinatorial study is also to identify markers of disease, develop diagnostic tools and even design new therapeutic agents.

Keywords: Pharmacology, Clinical Microbiology, Pathological Applications, Microorganisms, Antimicrobial Study, Biochemistry.

Biography

Prayash Chakraborty, born on 29th April 2003 is a II-year MBBS (Bachelor of Medicine & Surgery) student at Jagannath Gupta Institute of Medical Sciences & Hospital in Calcutta, West Bengal, India. Has qualified in National Level Entrance Test (NEET) for getting himself admitted in MBBS course. At present course curriculum contains Pharmacology, Pathology and Microbiology. Already studied Biochemistry, Physiology and Anatomy in I-year course. Interested in "Interdisciplinary curriculum based studies at present pertaining into present methodologies of learning systems and want to pursue higher research in this specialization in near future.



MS. Samar Nafafaa* (M.A), Ms. Ranin Suliman (M.sc), Dr. Elena Bekovetsky (Ph.D.)

Ziv Medical Center, Safad, Isreal

Evaluation of complement proteins C3, C4, and CH50 in ICU patients with COVID-19: No clear correlation with disease severity

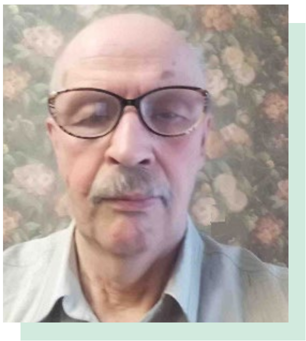
This study aimed to investigate the levels of complement proteins C3, C4, and CH50 in critically ill COVID-19 patients admitted to the Intensive Care Unit (ICU). The complement system plays a crucial role in the immune response to infections, contributing to pathogen clearance and inflammation. However, its involvement in the pathogenesis and severity of COVID-19 remains unclear. Some studies have suggested that excessive complement activation may contribute to severe disease outcomes, while others have reported conflicting results.

To explore this further, blood samples were collected from ICU patients diagnosed with COVID-19, and the levels of C3, C4, and CH50 were measured. The aim was to determine whether elevated levels of these complement proteins correlate with the severity of COVID-19 infection. The results demonstrated no consistent pattern of complement activation across all patients. While some patients exhibited increased levels of C3, C4, and CH50, others showed no significant elevation, indicating a lack of uniform complement activation in severe COVID-19 cases.

These findings suggest that complement activation alone may not be a major determinant of COVID-19 severity in critically ill patients. The variability observed in complement protein levels highlights the complex nature of the immune response in COVID-19, suggesting that multiple immunological and physiological factors contribute to disease progression. Furthermore, this study underscores the need for further research to explore other potential biomarkers and mechanisms that may better explain the heterogeneity in disease severity among COVID-19 patients. Future studies should investigate the interplay between complement activation and other immune pathways to provide a more comprehensive understanding of COVID-19 pathophysiology and to identify potential therapeutic targets for severe cases.

Biography

Samar Nafafaa is a medical laboratory scientist with over ten years of experience in clinical diagnostics, holds a bachelor’s degree in Medical Laboratory Sciences and a master’s degree in Medical Services and Pharma Management. Samar specializes in In Vitro Fertilization (IVF) and currently work at Ziv Medical Center in Safed. And, is part of the biochemistry laboratory and coordinate the immunology field within the chemistry lab. Her expertise includes biochemistry, immunology, and laboratory management. Samar Nafafaa is committed to enhancing diagnostic processes, improving patient care, and advancing laboratory science through continuous research and professional development.



Valery N. Belyaev

The private person, Ivanovo, Russian Federation

On a new approach to determining the ionization potential of molecules from spectroscopic data

A new on principle approach has been developed for determining the adiabatic ionization potential $I_o(MX)$ of polar $eM^{2+}X^-$ molecules with high accuracy (no worse than 0.02 eV) using spectroscopic data only. This approach is based on measurement of difference of Stark displacements $\Delta E^o=\frac{1}{2}\alpha'(\varepsilon')^{2-}\frac{1}{2}\alpha''(\varepsilon'')^2$ by internal field of X^- anion with strength $\varepsilon=e/r^2$ in $eM^{2+}X^-$ molecule of its electronic terms formed by non-bonding e electron orbitals located at M^{2+} on distance r_o from X^-. The molecular transition between the lowest non-bonding e electron orbitals observes in spectrum as the Rydberg series beginning $T_o(MX)$ displaced from an atomic line E(M) on $\Delta E^o=To(MX)–E(M)$ named by the optical shift which is immediately connected with the desired $I_o(MX)$ as follows from: $I_o(MX)=I_o(M)^-$Thus all magnitudes in formula for $I_o(MX)$ are found only from the MX, M and M^+ spectra. The adiabatic ionization potentials of MX molecules with evaluated upper limit of its error ±0.019 eV are presented below.

$$\frac{\alpha'}{\alpha''}=2-\frac{E(M^+)-E(M)}{I_o(M^+)-I_o(M)} \qquad \frac{T_o(MX)-E(M)}{\left[2-\frac{E(M^+)-E(M)}{I_o(M^+)-I_o(M)}\right]\left(\frac{r_o''}{r_o'}\right)^4-1}$$

Metal	Parameter	F	Cl	Br	J
Ca E(Ca)=15227.969 cm–1 E(Ca+)=25302.955 cm–1 Io(Ca)=6.113213 eV Io(Ca+)=11.8718 eV	r_o'', Å	1.955110(42)	2.43991097(15)	2.59635350(96)	2.83130(30)
	r_o', Å	1.958543(44)	2.420655(16)	2.568866(28)	2.78275(47)
	To(B2Σ+), cm–1	18833.136(52)	16855.144(10)	16383.113(15)	15716.7502(78)
	Io(CaX), eV	5.533	5.873	5.947	6.047
Sr E(Sr)=14573.478 cm–1 E(Sr+)=24115.92 cm–1 Io(Sr)=5.694901 eV Io(Sr+)=11.0302 eV	r_o', Å	2.0785831(17)	2.5787221(18)	2.7375185(54)	2.97578928(43)
	r_o', Å	2.0833525(96)	2.559340(11)	2.709809(14)	2.929918(11)
	To(B2Σ+), cm–1	17264.1418(24)	15725.1112(18)	15355.7795(34)	14820.1619(7)
	Io(SrX), eV	5.257	5.523	5.581	5.661
Ba E(Ba)=9315.351 cm–1 E(Ba+)=5274.337 cm–1 Io(Ba)=5.2117053 eV Io(Ba+)=10.004 eV	r_o'', Å	2.16217706(38)	2.68540585(24)	2.84657693(35)	3.0867767(41)
	r_o', Å	2.20723(10)	2.7367397(45)	(2.893±0.023)	3.1275903(48)
	To(B2Σ+), cm–1	14040.15(2)	11867.3380(20)	11325	10421.91246(54)
	Io(BaX), eV	4.587	4.879	4.956±0.02	5.074
Yb E(Yb)=18330.278 cm–1 E(Yb+)=28727.025 cm–1 Io(Yb)=6.25394 eV Io(Yb+)=12.184 eV	r_o'', Å	2.019182(98)	2.490915(13)	—	—
	r_o', Å	1.98967(40)	(2.4420.005)	—	—
	To(B2Σ+), cm–1	21073.33(50)	19938.4(33)	—	—
	Io(YbX), eV	5.872	6.040	—	—

It is proposed to make this approach by part of the spectroscopic studies along with the determination of other molecular parameters from the spectra: vibrational, rotational and electronic ones.

Biography

Valery Nikolayevich Belyaev, 73 years old, candidate of physical and mathematical sciences, graduated Ivanovo Institute for Chemistry and Technology, after worked in research laboratory under direction Prof. K.S. Krasnov, investigated the energetic of chemical and radiative processes in flames with additives of alkaline, alkaline earth, 3-d transitional and rare earth metals. Valery Nikolayevich is author about 80 articles and abstracts of conferences.

Notes:

BOOK OF ABSTRACTS

We wish to meet you again at our upcoming event

6th Edition of

Chemistry World Conference

June 2026 | Barcelona, Spain | Hybrid Event

https://chemistryworldconference.com/

Questions? Contact

Phone: +1 (702) 988 2320 | Whatsapp: +1 (640) 666-9566

e-mail: chemistry@magnusconference.com