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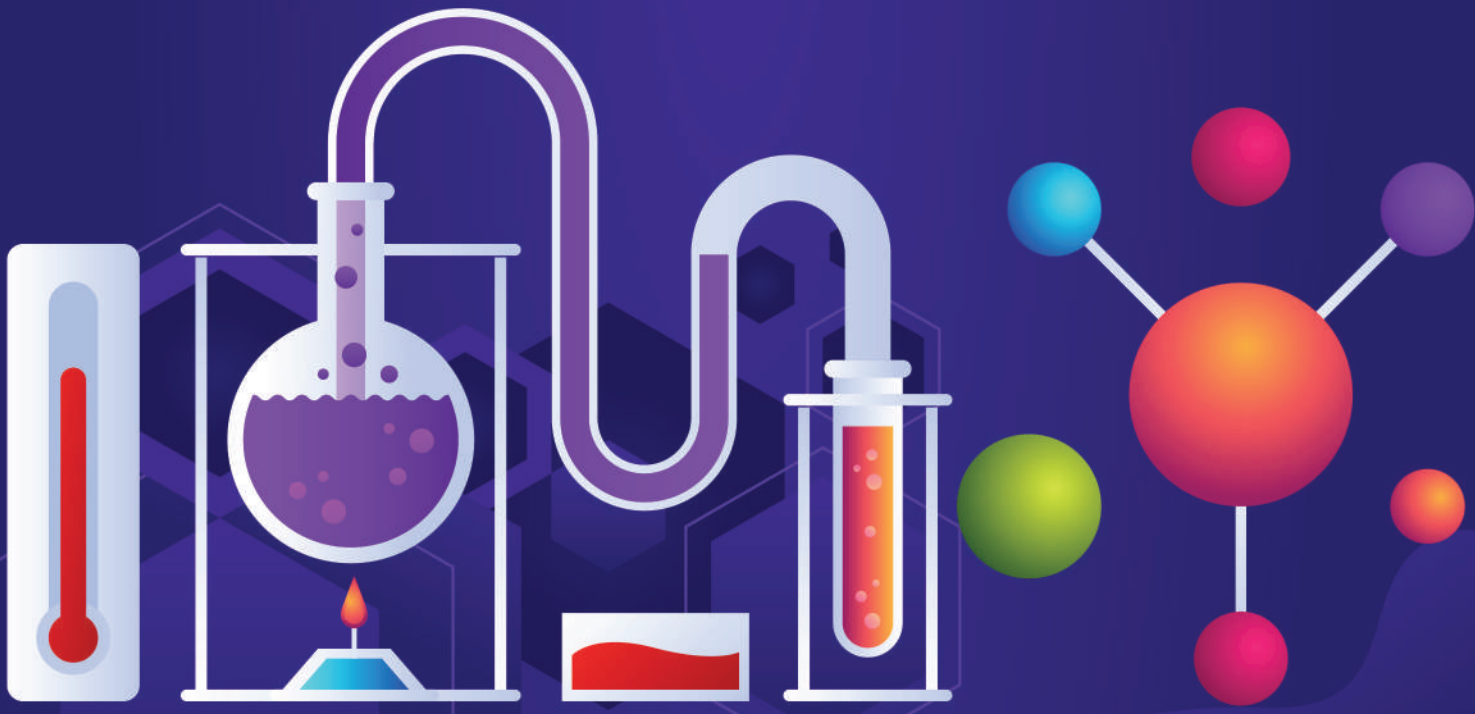
5th Edition of Advanced Chemistry World Congress

March 25-26, 2024 | Amsterdam, Netherlands



Adv. Chemistry 2024

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PROGRAM-AT-A-GLANCE >>

YOUR FIRST CHOICE FOR RESEARCH INGENUITY

ADV. CHEMISTRY 2024

DAY 1
MARCH 25, 2024

Scientific Program

08:00-08:45	**Registrations**
08:45-09:00	**Opening Ceremony**

Moderator: Giovanni Sansoe, *Gradenigo Hospital, Torino, Italy*

Topics: Analytical Chemistry | Industrial Chemistry | Agricultural Chemistry | Medicinal Chemistry | Chemical Engineering | Green Chemistry | Environmental Chemistry | Biochemistry | Organic Chemistry | Physical Chemistry | Geochemistry | Food Chemistry | Materials Science | Molecular Biology | Polymer Chemistry and Technology

Distinguished Speaker Talks

Session Chair	**Bourrié Guilhem,** *Académie d'agriculture de France & INRAE, France*
Session Chair	**Guy Vereecke,** *imec, Belgium*
09:00-09:20	**Title: Reactions, redox potential and kinetics with special relevance to geochemistry and life emergence** **Bourrié Guilhem,** *Académie d'agriculture de France & INRAE, France*
09:20-09:40	**Title: The surge in aseptic processing technology** **Stephen Scypinski,** *Stephen Scypinski Consulting LLC, USA*
09:40-10:00	**Title: Benefits and risks of sun exposure to maintain adequate vitamin D levels** **Suzanne Riskin,** *Nova Southeastern University, USA*
10:00-10:20	**Title: New viral diseases and new treatment options: The pharmacology of the non-classical renin-angiotensin system** **Giovanni Sansoe,** *Gradenigo Hospital, Torino, Italy*
10:20-10:40	**Title: The use of water structure breaking or making ions to control etching reactions in nanoconfined spaces** **Guy Vereecke,** *imec, Belgium*

Group Photo 10:40-10:50

Refreshment Break 10:50-11:05

11:05-11:25	**Title: Tris(β-ketoiminate) AlIII compounds as aluminium oxide precursors** **Erica N. Faria,** *University College London (UCL), UK*
11:25-11:45	**Title: Investigation of Runx1 as a new therapeutic target and the effects of its chemical inhibitors on cardiac function in a rat model of myocardial infarction** **Weihong He,** *Sichuan University, China*
11:45-12:05	**Title: Synthesis and evaluation of core-shell nanocomposites for the photodegradation of Liner Alkyl-benzene Sulfonate water contaminations** **Mohamed Ez-Dean Rashad Hassan,** *Port Said University, Egypt*
12:05-12:25	**Title: The structure-property-processing relationship for biocompatible and moldable silk fibroin nanofibrils** **Jen-Chang Yang,** *Taipei Medical University, Taiwan*
12:25-12:45	**Title: Low-temperature deposition of conductive copper through the design of molecular precursors** **Jingyan Wang,** *University College London (UCL), UK*
Group Photo 12:45-12:55	
Lunch Break 12:55-13:35	
Session Chair	**Bourrié Guilhem,** *Académie d'agriculture de France & INRAE, France*
Session Chair	**Guy Vereecke,** *imec, Belgium*
13:35-13:55	**Title: Computational studies on the photochemical reaction paths of cyclic nitrones and dinitrones** **Anjan Chattopadhyay,** *Birla Institute of Technology and Science (BITS) Pilani, India*
13:55-14:15	**Title: Production of extracellular enzymes by *Lentinula edodes* strains in solid state fermentation on lignocellulosic biomass sterilized by physical and chemical methods** **Ezequiel Marcelino Silva,** *Federal University of Tocantins, Brazil*
14:15-14:35	**Title: Palladium nanoparticles incorporated graphitic carbon nitride nanosheets for visible light catalytic reforming of biomass for hydrogen evolution** **Beena Mathew,** *Mahatma Gandhi University, India*
14:35-14:55	**Title: Single-nucleotide polymorphisms in MTHFR gene related to recurrent abortion** **Yasin Kareem Amin,** *Medical College, Erbil Medical University, Iraq*

14:55-15:15	**Title: Rotamerism, geometrical isomerism and intramolecular proton transfer in curcuminoids** **Francis A. S. Chipem,** *Manipur University, India*
15:15-15:35	**Title: Insights into the adsorption mechanism of graphene oxide functionalized WO_3 nanocomposite for removal of Cu(II) ions from aqueous solutions: Kinetics, equilibrium, thermodynamics and artificial neural network modelling** **Balasubramani Kavitha,** *C.P.A College, India*

Refreshment Break 15:35-15:50

15:50-16:10	**Title: Multitask learning for the segmentation of red blood cells in a sickle cell anemia diagnosis using efficient optimised efficient net model** **Princy Matlani,** *Guru Ghasidas Vishwavidyalaya (Central University), India*
16:10-16:30	**Title: Analysis of the mineralogical and chemical compositions of the laterization products of the parent rock of African major Bauxite deposits** **Nafiu Mohammed Zainudeen,** *Institute of Scientific and Technological information (INSTI), Council for Scientific and Industrial Research (CSIR), Ghana*
16:30-16:50	**Title: Subchronic toxicity study of herbal tea of Moringa stenopetala (Baker f.) Cudof. and Mentha spicata L. leaves formulation in Wistar albino rats** **Abinet Admas Alemneh,** *Saint Paul's Hospital Millennium Medical College, Ethiopia*
16:50-17:10	**Title: Protein folding problem: Enigma, paradox, solution** **Alexei V. Finkelstein,** *Russian Academy of Sciences (IPR), Moscow State University, Russia*
17:10-17:30	**Title: Development of a new PET tracer [68Ga]68Ga-DOTA-ECL1i to noninvasively track fibrotic changes in myeloproliferative neoplasms based on C-C Chemokine receptor 2 detection** **Silvia Migliari,** *Azienda Ospedaliero-Universitaria di Parma, Italy*

Panel Discussion

End of Day 1

DAY 2
MARCH 26, 2024

Scientific Program

07:40-08:25	**Registrations**
08:25-08:40	**Introduction**

Moderator: Giovanni Sansoe, *Gradenigo Hospital, Torino, Italy*

Topics: Analytical Chemistry | Industrial Chemistry | Agricultural Chemistry | Medicinal Chemistry | Chemical Engineering | Green Chemistry | Environmental Chemistry | Biochemistry | Organic Chemistry | Physical Chemistry | Geochemistry | Food Chemistry | Materials Science | Molecular Biology | Polymer Chemistry and Technology

Distinguished Speaker Talks

Session Chair	**Sharadha Sambasivan,** *Suffolk County Community College, USA*
Session Chair	**Beena Mathew,** *Mahatma Gandhi University, India*
08:40-09:00	**Title: Solubility of fluorite in concentrated electrolyte solutions at elevated temperatures: Implications to nuclear waste-form development and rare earth element (REE) extraction** **Yongliang Xiong,** *Sandia National Laboratories (SNL), USA*
09:00-09:20	**Title: Water quality evaluation and impact of nitrogen contamination** **Sharadha Sambasivan,** *Suffolk County Community College, USA*
09:20-09:40	**Title: Conformational changes of human stratum corneum lipids by effect of cyclic and linear siloxanes** **Krystyna Pieńkowska,** *Medical University of Gdańsk, Poland*
09:40-10:00	**Title: Montmorillonite-based chitosan nanocomposites as sustainable slow-release green fertilizers** **Punnama Siriphannon,** *King Mongkut's Institute of Technology Ladkrabang, Thailand*
10:00-10:20	**Title: Graphene assisted optical tweezers and its applications** **Yuquan Zhang,** *Shenzhen University, China*

10:20-10:40	**Title: Polyol-based extraction: A green approach to extract bioactive compounds for cosmetic and tropical products** **Nuntawat Khat-udomkiri,** *Mae Fah Laung University, Thailand*

Group Photo 10:40-10:50

Refreshment Break 10:50-11:05

11:05-11:25	**Title: Synthesis and molecular structure studies of Aluminium (III) complexes with β-ketoiminate and ethanolamine ligands** **Leonardo Santoni,** *University College London (UCL), UK*
11:25-11:45	**Title: Advanced insights into phenylpropene biosynthesis in *Ocimum basilicum* L.: The role of vermicompost form, dose, and application method** **İlker TÜRKAY,** *Kırşehir Ahi Evran University, Turkey*
11:45-12:05	**Title: Electrical conductivity, microstructures, chemical compositions, and systematic multivariable models to evaluate the effect of waste slag smelting (pyrometallurgical) on the compressive strength of concrete** **Ahmed Salih Mohammed,** *American University of Iraq Sulaimani, Iraq*
12:05-12:25	**Title: Tumor cell adhesion and metastasis signaling: Contribution of endothelium nitric oxide** **Fabiola Sánchez,** *Universidad Austral de Chile, Chile*
12:25-12:45	**Title: CdO nanostructures as acid-base bifunctional heterogeneous catalysts for making Coumarin-3- Carboxylic Acids at room temperature** **Rupinder Kaur,** *Indian Institute of Science Education and Research Mohali, India*

Group Photo 12:45-12:55

Lunch Break 12:55-13:35

Session Chair	**Beena Mathew,** *Mahatma Gandhi University, India*
Session Chair	**Jen-Chang Yang,** *Taipei Medical University, Taiwan*
13:35-13:55	**Title: Composition and characterisation of ancient lime mortar of 12th century temple, Alandi, India** **Sarvesh Singh,** *Reserve Bank of India Archives, India*

13:55-14:15	**Video-Presentation: Calcium element quantification model using a portable X-ray fluorescence unit** **Claudio Hernán González-Rojas,** *Universidad de Tarapacá, Chile*
14:15-14:35	**Title: Regulatory role of LexA in modulating photosynthetic redox poise and cadmium stress tolerance in the cyanobacterium, *Anabaena* sp. PCC7120** **Yogesh Mishra,** *Banaras Hindu University, India*
14:35-14:55	**Title: Green practices implementation for environmental sustainability by five-star hotels in Kampala, Uganda** **Alex Barakagira,** *Kyambogo University, Uganda*
14:55-15:15	**Title: Poly(amido amine) functionalized graphene oxide for enhancing properties of a polysulfone ultrafiltration membrane: Effect of Poly(amido amine) generation** **Ahmed Toky Yasir,** *Qatar University, Qatar*
15:15-15:35	**Title: Carboxymethyl cellulose for oil and gas field operations** **Hauwa Abubakar Rasheed,** *Nile University of Nigeria, Nigeria*
15:35-15:55	**Title: Monocyte HLADR and Immune Dysregulation Index as biomarkers for covid-19 severity and mortality** **Namrata P Awasthi,** *Dr. Ram Manohar Lohia Institute of Medical Sciences, India*
Refreshment Break 15:55-16:10	
16:10-16:30	**Title: The problem of relation between excess and absolute adsorption: Rigorous results** **Eduard Sergeevich Jakubov,** *Russian Academy of Sciences, Russia*
16:30-16:50	**Title: In quest of small molecules as dengue NS2B-NS3 protease inhibitor using in-silico molecular docking** **Deepali Mahir Nahar,** *St. John Institute of Pharmacy and Research, India*
16:50-17:10	**Title: How can ice emerge at 0°C and what do ice-binding proteins do?** **Alexei V. Finkelstein,** *Russian Academy of Sciences (IPR), Moscow State University, Russia*
17:10-17:30	**Title: Activation of inactive enzymes through biochemical and evolutionary approaches** **Eri Tabata,** *Kogakuin University, Japan*

17:30-17:50	**Title: *In-situ* and transported nickel-rich regolith in the Bavanat region, SW of Iran: Constraints from geochemistry and mineralogy** **Soqra Rasti,** *Shiraz University, Iran*
17:50-18:10	**Video-Presentation: Utilizing choline chloride-containing DESs to extract value-added compounds from tomato pomace and incorporating them into cosmetic emulsion formulations** **Liudmyla Khrokalo,** *Igor Sikorsky Kyiv Polytechnic Institute, Ukraine*

Panel Discussion

End of Day 2

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DISTINGUISHED SPEAKER TALKS

DAY 1

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ADVANCED CHEMISTRY WORLD CONGRESS

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Reactions, redox potential and kinetics with special relevance to geochemistry and life emergence

G. Bourrié[1,2] and **F. Trolard**[1,2]

[1]Académie d'agriculture de France, France
[2]INRAE, France

The aims of this study is to recall the evolution of ideas in the domain of redox reactions. Steel corrosion studies led Pourbaix (1949) to propose (Eh, pH) diagrams applied by Krumbein and Garrels (1952) to the classification of sediments. Many (Eh, pH) measurements however were not conclusive, as redox reactions are either sluggish or biologically mediated, which led Berner (1981) to discourage using (Eh, pH) measurements. But Fe(II)/Fe(III) appear to be electroactive at Pt electrode, so Eh measurements may be relevant in waterlogged environments where anaerobic / aerobic conditions alternate. Green rusts, first evidenced as corrosion intermediates, supposed since 1905 by Vyssotskii to be present in gleys were identified in hydromorphic soils by Trolard et al. (1996) and homologated as fougerite by IMA in 2007. This mineral is a key criterion in all soil taxonomies (World Reference Base) to define reducing conditions. It interacts with N cycle and many minor and trace elements, controls Fe in solution and is a precursor of ferric oxides and clay minerals. Stumm and Schulzberger (1992) showed that Fe(II)/Fe(III) standard potential can span the entire stability domain of water, depending on the exact nature of active compounds. At the lowest boundary, ferrous hydroxide can reduce water, oxidize into fougerite with hydrogen formation. This occurs in serpentinisation of oceanic crust bearing many hydrothermal springs considered by Russell (2020) as the cradle of life in Hadean ocean, with fougerite as "the seed of all life". As oxidation proceeds, fougerite oxidizes in ferric oxides, or ferric clay minerals, such as greenalite, present in banded iron formations (BIF), that are the main iron ores. Fougerite, as a layered double hydroxide, bears membrane-like properties that could have facilitated prebiotic evolution. Molecular phylogeny shows that active sites in some enzymes can be viewed as minerals "nested" by peptides (Milner-White, 2019).

Biography

Pr. Guilhem Bourrié made his Ph.D in Strasbourg (1976), after graduations as an agronomist and a geologist in Paris. He was scientist at INRA and a Professor in the Geosciences Department in Rennes University, then created the Soil and Water Geochemistry Department in Aix-en-Provence. He authored or co-authored over 200 scientific publications, 44 book chapters, edited 11 books in soil science, geochemistry and geomorphology. He contributed to the creation of the European Journal of Soil Science. He dedicated to the geochemistry of soil / water interactions, in acid forested soils, Al speciation, minerals equilibria, and Fe and trace metals dynamics in hydromorphic soils, under aerobic / anaerobic conditions, in soils submitted to large inputs of cattle manure, or intensive rice cropping. He cooperated on reclamation of salt-affected soils in Syria, Algeria and Tunisia and on metal toxicity in Chile. He is a member of the Académie d'agriculture de France.

The surge in aseptic processing technology

Stephen Scypinski

Stephen Scypinski Consulting LLC, USA

Aseptic processing, which is the manufacture of pharmaceuticals and biopharmaceuticals under sterile conditions, has seen a sharp rise over the past several years. Both Contract Manufacturing Organizations (CMOs) as well as pharmaceutical and biotechnology companies have expanded their aseptic processing capabilities. Several factors have led to this sharp increase. Firstly, the growing number of biologic entities in the clinic and commercialized have contributed to the need for additional aseptic capacity. Growth was also accelerated by the COVID-19 pandemic whereby companies such as Pfizer and Moderna scrambled to secure external manufacturing. These factors have driven CMOs to expand their capacity. However, this is not readily accomplished as an aseptic processing facility requires extensive qualification and validation prior to its use. Therefore, the industry recognizes that there is a capacity shortage. This presentation will discuss some of the challenges facing the pharmaceutical industry regarding aseptic processing as well as discuss trends in the aseptic area.

Biography

Dr. Stephen Scypinski is a semi-retired independent consultant in all areas of Chemistry, Manufacturing and Controls (CMC). He has spent over 30 years in the pharmaceutical industry and has worked at large pharma companies such as Johnson & Johnson, Hoffmann-La Roche and Bristol-Myers Squibb as well as small biotech and start-up companies. Dr. Scypinski has played a leading role in bringing over 60 products to market including the blockbuster drugs ELIQUIS, FARXIGA, OPDIVO, and ENHERTU. He is the Editor-in-Chief of the Journal of Pharmaceutical Innovation and co-editor of the text Handbook of Pharmaceutical Analysis. Dr. Scypinski is an adjunct professor at Duquesne University School of Pharmacy.

Benefits and risks of sun exposure to maintain adequate vitamin D levels

S.I. Riskin and **J.R. Raymond-Lezman**

Dr. Kiran C. Patel College of Osteopathic Medicine Tampa Bay Regional Campus, Nova Southeastern University, USA

Vitamin D is a hormone that can be generated in the skin upon ultraviolet light exposure or ingested through supplementation. Vitamin D deficiency may have numerous deleterious effects on health. Sun avoidance strategies should be avoided due to the unwanted health risks associated with hypovitaminosis D. We present an objective investigation of the benefits and risks of using sun exposure to increase vitamin D levels and how it impacts human health. A review of the literature was conducted using Embase and PubMed to examine the relationship between UV exposure, vitamin D levels, health benefits, and risks.

UV exposure is the primary method of boosting serum vitamin D levels, which accounts for numerous health benefits. Higher levels of vitamin D are associated with protection against cancer development, including melanoma. Latitude, season, skin color, and sun protection determine UV absorption and vitamin D production. Public health sun protection guidelines decrease the incidence of skin cancer, but sun avoidance can cause hypovitaminosis D. Serum vitamin D levels less than 16 nmol/L increase morbidity through increased non-cutaneous disease. Sun protection strategies should still be implemented to reduce skin cancer, and sunscreen only minimally lowers vitamin D production. Vitamin D deficiency can increase chronic diseases and cancer, while adequate vitamin D levels can help prevent them. UV exposure and vitamin D production are dependent on many factors. Increasing UV exposure without causing sunburn maximizes vitamin D production.

Biography

Suzanne I. Riskin, M.D. is an Assistant Professor of Internal Medicine and Foundational Sciences at Nova Southeastern University Dr. Kiran C. Patel College of Osteopathic Medicine (NSU KPCOM), Tampa Bay Regional Campus (TBRC). She completed B.A. from The University of Pennsylvania and M.D. from The University of Miami, Miller School of Medicine.

Dr. Riskin has had grant and scholarship opportunities and is a published book chapter author. Research interests include medical education, preventative health, cancer prevention, primary care, combating health inequities, and medical humanities.

Dr. Riskin is a poster judge at local, state and national competitions. Dr. Riskin presented at Continuing Medical Education (CME) credit conferences on medical education and preventative health.

Dr. Riskin is experienced with a demonstrated history of working in the higher education industry. She enjoys free time floating down a river in a kayak or cooking a great meal. You can reach her at sriskin@nova.edu.

New viral diseases and new treatment options: The pharmacology of the non-classical renin-angiotensin system

Giovanni Sansoe[1] and **Manuela Aragno**[2]

[1]Division of Gastroenterology, Humanitas Institute, Gradenigo Hospital, Torino, Italy
[2]Department of Clinical and Biological Sciences, University of Torino, Italy

All strains of SARS-CoV-2 and previously described SARS-CoV and MERS-CoV bind to ACE2, the cell membrane receptor of these β-coronaviruses. Monocarboxypeptidase ACE2 activity stops upon viral entry into cells, leading to inadequate tissue production of angiotensin 1-7 (Ang1-7). Acute lung injury due to human respiratory syncytial virus (hRSV) or avian influenza A H7N9 and H5N1 viruses is also characterized by significant downregulation of lung ACE2 and increased systemic levels of angiotensin II (Ang II). Restoration of Ang1-7 anti-inflammatory, anti-fibrotic, vasodilating, and natriuretic properties was tried at least in some Covid-19 patients through i.v. infusion of recombinant human ACE2 or intranasal administration of modified ACE2 protein, with inconsistent clinical results. Conversely, use of ACE inhibitors (ACEis), which increase ACE2 cell expression, seemed to improve the prognosis of hypertensive patients with Covid-19.

To restore Ang1-7 tissue levels in all these viral diseases and avoid the untoward effects frequently due to ACE2 systemic administration, a different strategy may be hypothesized. Experimentally, when metallopeptidase inhibitors block ACE2, neprilysin (NEP), highly expressed in higher and lower airways, starts cleaving angiotensin I (Ang I) into Ang1-7. A discerning use of ACEis should be made in normo-hypertensive pneumonia patients to block ACE-dependent Ang II synthesis and Ang1-7 degradation into angiotensin 1-5; at the same time, i.v.-infused Ang I, which is not hypertensive provided ACE is inhibited, may become the primary substrate for local Ang1-7 synthesis by ubiquitous NEP. NEP could replace inadequate tissue Ang1-7 production if Ang I were freely available, in coronavirus disease as well as in atypical pneumonia caused by avian influenza viruses and hRSV. Moreover, inhibitors of chymase, serine endopeptidase responsible for 80% of Ang II forming activity in tissues and vessel walls, could protect patients with atypical pneumonia from Ang II–mediated microvascular damage without reducing arterial blood pressure.

Biography

Giovanni Sansoe is Internationally recognized expert in the pharmacology of classical and non classical renin-angiotensin system (RAS) in hepatic, renal and viral diseases. Main author of the recently published reviews: "COVID-19 and liver cirrhosis: focus on the non-classical renin-angiotensin system and implications for therapy", *Hepatology* 2021; 74 (2): 1074-1080, and "New viral diseases and new possible remedies by means of the pharmacology of the renin-angiotensin system", *Journal of the Renin-Angiotensin-Aldosterone System* 2023, Article ID 3362391; https://doi.org/10.1155/2023/3362391. The above imply considerable knowledge of the newly-described mechanisms of disease progression due to all pathways of the renin-angiotensin system, and vision of future therapeutic development in the following disciplines: hepatology, virology, nephrology, hemodynamics, cardiology, biochemistry and pharmacology.

4-time invited speaker at the annual meetings of the American Association for the Study of Liver Diseases (AASLD) (in 2004, 2006, 2013, 2014).

8-time invited speaker at the Digestive Disease Week (DDW, annual meeting of the American Gastroenterological Association) (in 2003, 2004, 2009, 2012, 2018).

Assistant professor, Division of Gastroenterology, Humanitas Institute, Gradenigo Hospital, Torino, Italy, from 1998 to 2023.

2011-2014. Scientific Consultant to Shire (pharmaceuticals): design, data collection and analysis of research protocols dealing with diuretic effects of different α-adrenergic and aquaretic agents in experimental cirrhosis.

June 2008-November 2008 (on leave from Gradenigo Hospital). Clinical Associate Professor in Hepatology (University of Calgary, Alberta, Canada).

July 2004-June 2005 (on leave from Gradenigo Hospital). Clinical Fellowship (University of Toronto, Ontario, Canada) working in the Department of Medicine of the Toronto General Hospital under the supervision of Prof. Florence Wong.

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The use of water structure breaking or making ions to control etching reactions in nanoconfined spaces

Guy Vereecke, Kurt Wostyn and **Efrain Altamirano Sanchez**

imec, Belgium

In semiconductor manufacturing, new generations of devices have entered the nano-world, with critical dimensions of the order of 10 nm. Moreover, new transistor geometries are vertical, with the generation of 1-D and 2-D nano-confined spaces. While many process steps are still performed using aqueous chemistries, e.g. wet etching of materials for patterning and wet cleaning of surfaces. Recent studies have shown that nano-confinement is affecting all the steps in a wet process, from wetting to chemical reactions, rinsing and drying.

Water structure modification by dissolved ions has been studied by Marcus (2009) for bulk solutions. Marcus published a classification of ions as structure breaking or making, which was tested using an ATR-FTIR technique developed by us (see Figure 1) in 32 nm wide nanochannels.

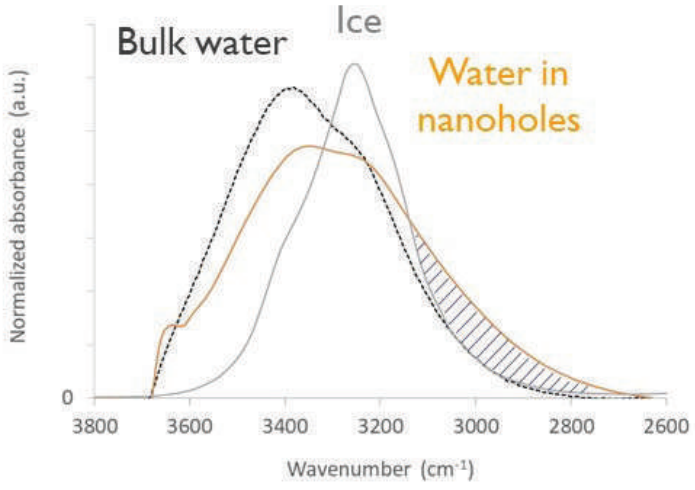

Figure 1: The FTIR OH stretching band of bulk water, ice, and water in nanoholes (diameter of 20 nm, depth of 300 nm). The spectra were obtained by ATR-FTIR, but for ice that was from literature. The hashed area indicates the structured water in nanoholes

We found that the ranking of ions, $Br^- > I^- > Cl^- > SO_4^{2-}$ as structure breaking, and $Fe^{2+} > Co^{2+} > Ca^{2+}$, as structure making, was in good agreement with Marcus Classification, differing only by the order of Br^- and I^-. The use of water structure breaking or making ions was studied to control an etching reaction in the FinFET fabrication flow. A gap fill oxide is used to fill the space between the Si fins that needs to be recessed to define the height of the fin trench. However, with the used oxide, the eth rate depends on fin spacing. This dependency could be suppressed for a gap of 15 nm width by adding structure-making cations of TPAH (tetra-propyl ammonium hydroxide) in HF mixtures. The pro's and con's of this approach will be reviewed.

Biography

Guy Vereecke holds a M.S. degree and a Ph.D. degree in Materials Sciences from the Université Catholique de Louvain (UCL), Louvain-La-Neuve, Belgium. In 1993, he joined the Ultra Clean Processing group of the Interuniversity Microelectronics Center (imec), where he is now a Principal Member of the Technical Staff in the Surface and Interface Processing group. He is author or co-author of more than 110 journal papers, 160 conference presentations, 5 book chapters, and 8 patents on surface analysis, gas phase corrosion and contamination, vapor phase cleaning, UV-assisted cleaning, laser cleaning, megasonic and spray cleaning of nano-particles and damaging of structured wafers, post-CMP cleaning, and wet strip and characterization of post-etch photoresist and residues. His H-index is 18. His current research topics are in wet processing of high aspect ratio nanostructures (wetting, cleaning, etching, rinsing and drying).

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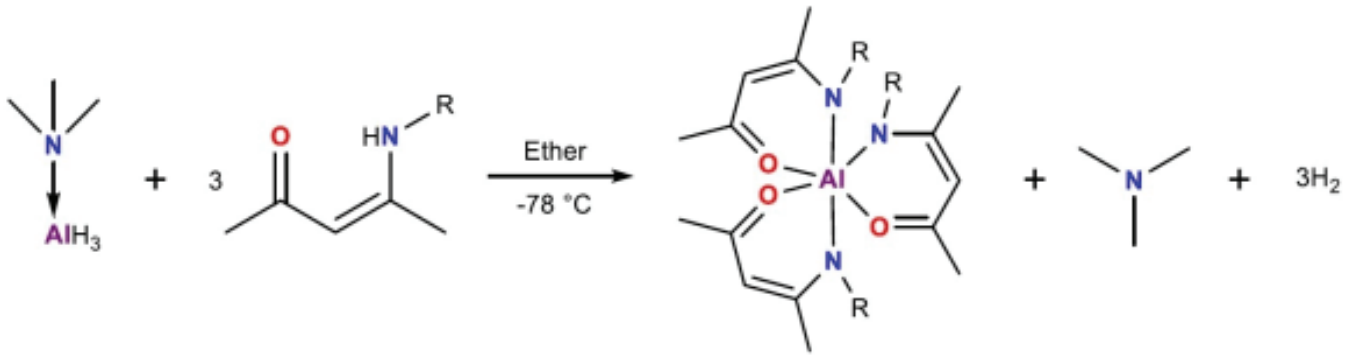
Tris (β-ketoiminate) AlIII compounds as aluminium oxide precursors

E. N. Faria, S. P. Douglas, S. Mrig, Y. Zhou, L. Santoni, A. J. Clancy and **C. E. Knapp**

Department of Chemistry, University College London, UK

Chelating ligands are well established in the field of metal-organic chemistry. Among these ligands,[1–3] conjugated six-membered ring chelates such as β-diketonates or "acacs" and β-ketoiminates or "acnacs" have been widely used. There has been particular interest in these ligand systems for use as precursors over the last few decades to deposit thin films of metal-based functional materials.[4–8]

The reduced number of examples of tris(β-ketoiminate) aluminium complexes described in the literature, with only three complexes previously reported,[9–11] prompted us to investigate the accessibility of such compounds through ligand substitution reactions.[12] The decomposition profile (200 – 350°C) of octahedrally coordinated tris(β-ketoiminate) aluminium complexes of the type [Al(MeCN(R)CHC=OMe)$_3$], can be tuned by varying the R substituents in the ligands. The complexes are derived from the reaction of trimethylamine alane (TMAA) and a series of N-substituted β-ketoiminate ligands (R-acnacH, R = Me, Et, ^{i}Pr, Ph) with varying R-substituents sizes. When the more sterically encumbered ligand (R = Mes) was used, the Al atom became five-coordinate, therefore representing the threshold to octahedral coordination around the metal in these types of compounds. Compound 1 (R = Me) has been used as a single source precursor for the deposition of Al_2O_3. Thin films were deposited *via* aerosol assisted chemical vapour (AACVD) with toluene as the solvent and were analysed using SEM, EDX and XPS.



Biography

Erica received her undergraduate degree from Universidade Federal de Minas Gerais, in Brazil. Following that, she obtained her DPhil at the University of Oxford (UK) and has recently join the Knapp group, as a Postdoctoral Research Associate. Her work in the group is focused on the synthesis of an array of aluminium complexes to be applied as precursors to functional materials.

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Investigation of Runx1 as a new therapeutic target and the effects of its chemical inhibitors on cardiac function in a rat model of myocardial infarction

Weihong He[3], Hengshu Chen[1], Si Wang[2], Xiaoling Zhang[2], Xing Hua[1], Meng Liu[1] and **Simiao Wu[1]**

[1]Department of Neurology, West China Hospital, Sichuan University, China
[2]Department of Cardiology, West China Hospital, Sichuan University, China
[3]Department of Physiology, West China School of Basic Medical Sciences and Forensic Medicine, Sichuan University, China

Myocardial infarction (MI) is a leading cause of death on a global scale. MI causes adverse changes in the architecture and function of the heart, referred to as cardiac remodelling. Progression of cardiac remodelling leads to heart failure and is linked to increased deaths or hospitalizations. Therefore, new therapeutic targets are urgently needed to prevent cardiac remodelling among patients with MI. Runt-related transcription factor-1 (RUNX1) is a member of the core-binding factor family of transcription factors and is intensively studied in hematopoietic field. Recent evidence shown that RUNX1 has a critical role in cardiomyocytes after MI and increased RUNX1 expression under pathological conditions leads to decreased cardiac contractile function. The previous study performed with a cardiomyocyte-specific Runx1-deficient mouse reveal that reducing RUNX1 function preserves myocardial contractility and prevents adverse cardiac remodeling after MI and therefore identifies RUNX1 as a new target for preventing adverse cardiac remodeling. The present study sought to investigate whether a small molecule inhibitor of Runx1 (Ro5-3335) can preserve cardiac contractile function following MI in rats. In this work MI was surgically induced in rats by performing coronary artery ligation and echocardiography was performed after MI to assess cardiac contractile function. Here we demonstrate that cardiac systolic function, as assessed by fractional shortening, decreased in control rats. In contrast, rats treated with Ro5-3335 demonstrated a markedly preserved fractional shortening that was 128% of the control rats at 1 week after MI (39.1±1.4% versus 30.6±2.9%; $P<0.05$). Heart samples after MI were collected and analyzed with mass spectrometry. Data-independent acquisition proteomics demonstrated that there were 524 down-regulated proteins and 24 up-regulated proteins in rat hearts treated with Ro5-3335 relative to control hearts. Our findings confirm the translational potential of RUNX1 as a new therapeutic target of MI and suggest that RUNX1 inhibitors could offer a potential therapy to counteract the effects of adverse cardiac remodelling.

Biography

Weihong He is a principal investigator and associate research fellow (associate professor) at the Department of Physiology, West China School of Basic Medical Sciences and Forensic Medicine, Sichuan University. Weihong obtained a MD (2012) at West China School of Medicine & West China Hospital, Sichuan University, and completed a PhD (2017) at the BHF Glasgow Cardiovascular Research Centre, University of Glasgow. Weihong was associate professor at Jining Medical University (2018-2020). Since 2020, Weihong has led a research group to study the pathophysiology of cardiovascular diseases and to investigate novel therapeutic drugs for the treatment of myocardial infarction at Sichuan University. He also teaches physiology and mentors both national and international students. Weihong has expertise in a number of methodologies which span the level of biochemistry, cell biology, isolated heart, and whole animal *in vivo* disease models.

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Synthesis and evaluation of core-shell nanocomposites for the photodegradation of Liner Alkyl-benzene Sulfonate water contaminations

Mohamed Ez-Dean Rashad Hassan, Mai E.S. Barakat and **Elsherbiny H.E. Yosef**

Port Said University, Egypt

Linear Alkyl-benzene Sulfonate surfactants (LAS) are a major pollutant source of sewage and wastewater. They trigger severe impact on the environmental fauna and flora. Current research explores the synthesis of three different core-shell nanocomposites (CSNCs) containing titania with conductive copolymers through an *in-situ* inexpensive oxidative polymerization technique. The fabricated CSNCs were evaluated for the photocatalytic degradation of LAS water contaminations.

The selected CSNCs investigated for this study were the TiO_2/poly(aniline-co-pyrrole) and TiO_2/poly(aniline-co-3-Me-thiophene) as well as the TiO_2/terpolymer (aniline-pyrrole-m-aminobenzoic acid). The structure of the formed nanocomposites was confirmed by varied characterization spectroscopy. The core-shell structure of the nanocomposites was confirmed by Scanning Electron Micrographs and Transmission Electron Microscopy.

The CSNCs exhibited intensive photo catalytic degradation efficacy toward LAS under visible light exposure in comparison with the exposure in their absence. The significant effectiveness of these nanocomposites in photodegradation of LAS under visible light is due to the synergetic effect of the conductive polymers and titanium oxide. A photodegradation mechanism was explained, justified, and presented in a clarifying diagram.

Assessment of photodegradation affecting parameters showed that the optimum photodegradation conditions would be attained at reasonably neutral pH, with nanocomposite dose in the range 100-150 mg/L, the initial concentration of LAS contamination would be advantageous to be controlled within the 10-100 mg/L range and the sun-light exposure of ten hours.

The presented approach implies that an effective, economical low-cost, and environmentally friendly one-pot synthetic technique was achieved to produce novel CSNCs, that have high potential for wide scale field and industrial applications and high potential as LAS photodegradation agents.

Biography

Dr. Mohamed Ez-Dean Rashad Hassan is a distinguished academic with a rich history in the field of chemistry and higher education administration. He earned his Ph.D. from the University of Manitoba, Canada, in 1976, following an M.Sc. from Azhar University in 1971 and a B.Sc. from Ain Shams University in 1965. Dr. Hassan's career includes notable roles such as Chemistry Professor at Port-Said University since 2004, a Visiting Professor at the University of Toronto in 2000, and Vice President of Academic & Student Affairs at South Valley University from 1997 to 2004.

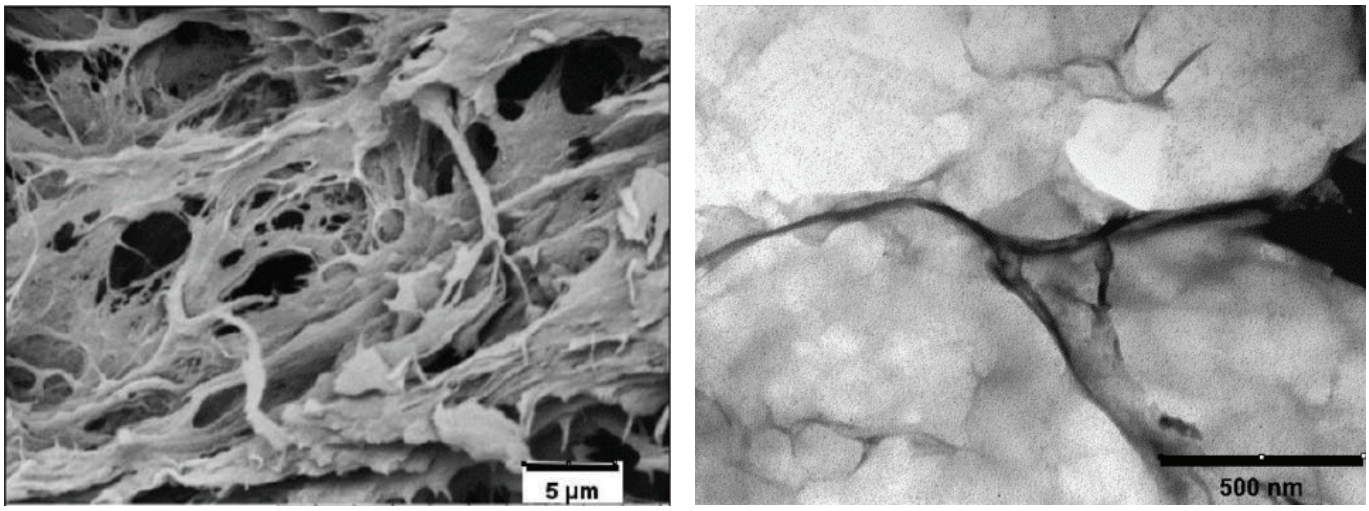
His extensive international experience encompasses positions like Visiting Professor in Jordan and Research Associate at Texas University, Kansas University, and the University of Western Ontario. Dr. Hassan's commitment to education and leadership is underscored by his participation in the Executive Management Training Program for University Administrators by The Bi-national Fulbright Commission in 2000.

The structure-property-processing relationship for biocompatible and moldable silk fibroin nanofibrils

J.C. Yang[1], Y.T. Wu[1], L.Y. Chang[1], P.W. Lu[2] and **C.C. Lin[3]**

[1]Graduate Institute of Nanomedicine and Medical Engineering, College of Biomedical Engineering, Taipei Medical University, Taiwan
[2]Division of Gastroenterology and Hepatology, Department of Internal Medicine, Shuang Ho Hospital, Taipei Medical University, Taiwan
[3]Institute of Organic and Polymeric Materials, National Taipei University of Technology, Taiwan

It is well known that silk would degrade prior to melting when subjected to thermal processing due to existence of β-pleated sheet nanocrystallites. The objectives of this study were to prepare and investigate the structure-property-processing relationship for moldable silk fibroin nanofibrils (SFNFs). Unlike a conventional dialysis/freeze-drying/milling process, SFNFs were prepared by a novel shear-induced phase-separation method. The SEM and TEM morphology of the resulting SFNFs were shown in Figure 1. And the particle size distribution, protein secondary structures, and crystalline structures of the resulting SFNFs were respectively investigated by laser diffraction (LD), Fourier-transform infrared (FTIR) spectroscopy, and x-ray diffraction (XRD) deconvolution analyses. *In vitro* hemolysis ratios, biocompatibility, and sensitization tests were carried out. Compared to dialyzed/freeze-dried/milling SF, the harvested SFNFs revealed high surface area in morphology. Shear-induced hydrogen bonding, crystallization, and phase separation tended to give the SFNFs a high crystalline index (CI) and degree of crystallinity (DC). The test results of toxicity and skin sensitization were both negative. The hemolysis ratio of SFNFs was classified as being non-hemolytic (< 2%). The high biocompatibility and of SFNFs revealed their potential biomedical applications.



(a) SEM (b) TEM

Figure 1. The (a) SEM and (b) TEM of SF nanofibrils prepared by shear-induced phase separation.

Biography

Jen-Chang Yang is a professor at the Graduate Institute of Nanomedicine and Medical Engineering at Taipei Medical University and also a joint-appointment professor at the School of Dentistry, the International Ph.D. Program in Biomedical Engineering and, the TMU Research Center of Biomedical Devices. He has a Ph.D. in Polymer Engineering from the University of Akron, USA. He has been working at Taipei Medical University since 2007, and has served as the vice dean of the College of Biomedical Engineering since 2019. His research interests include oral biomaterials, medical devices, silk protein, biomimetic materials, bioceramics, nanofiber technology, ionotronic hydrogels and weight management hydrogels. He has published more than 100 research papers and has participated in many projects related to nanomedicine and biomedical engineering.

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Low-temperature deposition of conductive copper through the design of molecular precursors

J. Wang and **C. Knapp**

Department of Chemistry, University College London (UCL), UK

Printed electronics have been widely used in various fields, from gas sensors to cloth tagging,[1,2] due to the feature of portability. Economical, flexible and compact electronic devices have become an important synthetic target as the market for printed electronics continues to expand. However, the high processing temperature of conductive inks has limited their industrial usage and application on low-cost flexible substrates. Lowering the decomposition temperature of conductive inks during the sintering process would enable printing on more temperature-sensitive materials.[3] Copper is a cost-effective metal with high conductivity and holds promise for use in printed electronic films.[4] Notably, alkanolamine has been known as both ligand and solvent to be added to copper precursors, enhancing solubility and reducing decomposition temperature.[5]

In this study, we describe the successful development of two copper metal-organic decomposition precursors using aminoethanol and aminopropanol as ligands. Through the reaction of copper (II) formate with excess alkanolamines, tris-coordinated copper precursor ions, $[CuL_3]$ each with a formate counter-ion, were isolated (Figure 1.). Their thermal decomposition mass spectrometry profiles were measured to assess their suitability for use in inks. Thermal gravimetric analysis showed both complexes decomposed at a temperature of <150°C, indicating that they are viable for printing on flexible substrates. Spin coating and inkjet printing are used to deposit highly conductive copper devices interconnected onto paper and polyimide substrates, and also for the production of functioning circuits that can power light-emitting diodes. The connections between precursor structure, decomposition profile and deposition properties are discussed with the aim of improving the rational design of precursors for low-temperature sintering.

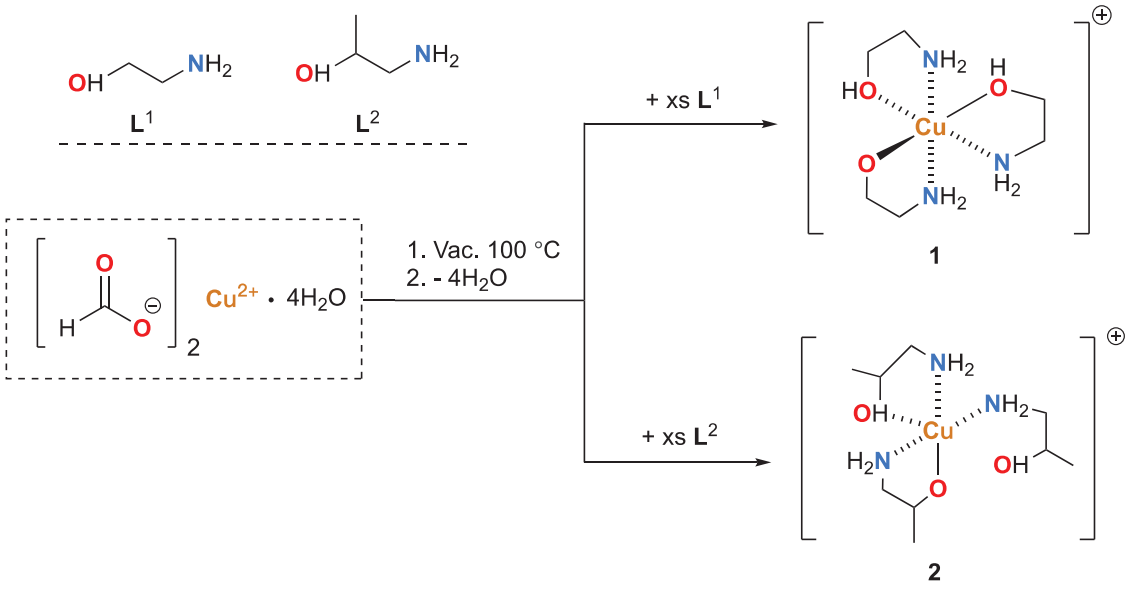

Figure 1 Synthetic routes to compounds 1 and 2. Formate counter ions omitted for clarity.

Biography

Jingyan is a second-year PhD in Knapp's group at UCL. The group focus on the synthesis, isolation and structural characterisation of highly air/moisture sensitive compounds and their subsequent use as precursors to materials. Her PhD research is focused on the design of precursors such that their decomposition can be fine-tuned. By adding various ligands to the precursors, the decomposition temperature can be lowered. She specialises in copper complexes that can be formulated into conductive inks and be used to inkjet print highly conductive tracks for use in flexible electronics.

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Computational studies on the photochemical reaction paths of cyclic nitrones and dinitrones

Anjan Chattopadhyay

Department of Chemistry, Birla Institute of Technology and Science (BITS) Pilani, India

Experimental studies on the photochemistry of methyl-substituted pyrroline 1-oxides, 2H-imidazole-1-oxides and 2H-imidazole-1,3-dioxides have been reported long back. However, the actual mechanisms leading to their photoproducts were not known for many years. In the last one decade, our group has thoroughly investigated and revealed these photochemical reaction paths through studies on their ground (S_0) and excited (S_1 and S_2) states using high level quantum mechanical calculations. In each case, photo-excitation of the cyclic N-oxide was found to form the photoproduct oxaziridine through a low-lying S_0/S_1 conical intersection (CI). The oxaziridine geometry consists of a heterocyclic CNO ring, slightly twisted upward or downward with a lone pair on nitrogen. The 2H-imidazole-1,3-dioxide systems were found to be involved in a 2-step photo-process, each step involving a low-lying conical intersection (S0/S1) which finally forms *trans* and *cis* dioxaziridines. Though the oxaziridine photo-conversion pathways of all these cyclic *N*-oxides are not significantly different, stabilities of these photoproducts are not similar and subsequently led to other products, in few cases. The oxaziridine obtained from DMPO and 3-Me DMPO (DMPO= 5,5-dimethyl-1-pyrroline 1-oxide) were less stable and found to convert easily to lactam through a [1,2]-H shift while the same for 2-Me DMPO (no H at 2-position) has to overcome a huge barrier to form this cyclic amide. This is in line with the experimental results which reported that heating at 300°C is required to form lactam in the latter case while this conversion is easier in the other two cases. Some other methyl-substituted pyrroline 1-oxides were reported to form multiple products (pyrroline, *N*-acetyl azetidine) on prolonged photo-irradiation and our computational studies were able to track all these reaction paths. The two diastereomeric dioxaziridines obtained as photoproducts from 2H-imidazole-1,3-dioxides were more stable than their oxaziridines where the latter can give back the parent dinitrone systems under heating. Overall, these studies have addressed most of the unanswered questions related to the photochemistry of these cyclic systems. Currently, our group is involved in exploring the photo-isomerization pathways of few other categories of important cyclic nitrone systems.

Biography

Dr. Anjan Chattopadhyay is working as a Professor in the Department of Chemistry, BITS-Pilani, K. K. Birla Goa Campus, Goa, India. His area of research expertise is computational chemistry and he primarily works on the photochemical and photophysical processes of organic molecules. His group is actively involved in exploring the photo-isomerization paths of nitrone compounds and crown ethers. He has contributed in the field of linear polyene photo-isomerizations, as well. Recently, his computational group has also explored the mechanism of alkali metal ion-initiated crown ether formation processes. His collaborative work with the experimental organic chemistry groups includes computational studies on the fluorescence of different types of organic molecules and their quenching processes.

Production of extracellular enzymes by *Lentinula edodes* strains in solid state fermentation on lignocellulosic biomass sterilized by physical and chemical methods

Ezequiel Marcelino Silva[1] and **Adriane Maria Ferreira Milagres**[2]

[1]Federal University of Tocantins, Brazil
[2]University of São Paulo, Brazil

Two methods of sterilization of lignocellulosic biomass were performed in this study. Eucalypt waste (EW) supplemented with rice bran (RB) was added in the proportions 80:20 and 90:10 in dry weight. The compositions were sterilized by physical method (autoclaving) and by chemical method (H_2O_2). The production of extracellular enzymes by *Lentinula edodes* strains was compared within the two methods. Inactivation of catalase present in RB was achieved with 250 mM H_2O_2. The H_2O_2 concentration was increased to 750 mM to ensure catalase inactivation and elimination of contaminating microorganisms in the EW: RB compositions. The use of H_2O_2, when compared by physical method, favored high production of hydrolytic enzymes such as endoglucanase (1,600 IU/kg), two-fold higher, β-glucosidase (1,000 IU/kg), five-fold higher, xylanase (55,000 IU/kg), three-fold higher and β-xylosidase (225 IU/kg), similar results. Oxidative enzymes, MnP and laccase, were produced within a different profile between strains, with shorter times for laccase (2,200 IU/kg) by SJC in 45 days and MnP (2,000 IU/kg) by CCB-514 in 30 days. High production of extracellular enzymes is achieved by the use of the chemical method of sterilization of lignocellulosic biomass, in addition to no energy consumption, this process is carried out in a shorter execution time when compared to the physical process. The use of H_2O_2 in sterilization does not produce toxic compounds from the degradation of hemicellulose and cellulose such as furfural and hydroxy-methyl-furfural that cause inhibition of microorganisms and enzymes. The residual solid load after enzyme extraction has much less lignin in composition and a high cellulose content that can be converted into glucose by enzymatic hydrolysis to produce bioethanol.

Biography

Ezequiel Marcelino Silva is graduated in Chemical Industrial Engineering at the School of Engineering of Lorena – University of São Paulo (USP). Master and PhD in Industrial Biotechnology from the School of Engineering of Lorena (EEL-USP) developing research on biodegradation of lignocellulosic biomass in solid state fermentation by basidiomycetes, evaluating the production of extracellular enzymes, mycelial growth by ergosterol extraction, fruiting yield and protein content in basidiomes. Post-doctorate in Molecular Biotechnology at the University of Brasília developing Alcoholic Fermentation of cassava starch by genetically modified Saccharomyces cerevisiae. Currently, Associate Professor I at the Federal University of Tocantins, teaching subjects such as Biotransformation of Organic Compounds, Enzymology and developing research related to the conversion of lignocellulosic biomass from agro-industrial waste by basidiomycetes in solid state fermentation for the production of extracellular enzymes, pre-treatment of lignocellulosic biomass with diluted acids, as well as biological (white rot fungi) and enzymatic hydrolysis for bioethanol production.

Palladium nanoparticles incorporated graphitic carbon nitride nanosheets for visible light catalytic reforming of biomass for hydrogen evolution

Beena Mathew, Neenamol John and **Chinnu R Thara**

School of Chemical Sciences, Mahatma Gandhi University, India

Photocatalytic H_2 production has become of paramount importance due to the depletion of fossil fuels and environmental contaminants. Biomass photoreformation is a revolutionary and distinctive method for both sustainable H_2 production and biomass valorization with limitless solar energy. However, this sustainable approach is typically associated with harsh reaction conditions, inadequate selectivity, and a limited amount of biomass conversion. Porous ultra-thin g-C_3N_4 carbon nitride nanosheets decorated with small Pd nanoparticles ((PdNPs < 5nm) were fabricated and their exceptional application in photocatalytic biomass reforming was investigated. The nanocomposites synthesis involves two-steps: (i) primarily thin g-C_3N_4 nanosheets were prepared with the thermal exfoliation method, and (ii) thiol-capped Pd nanoparticles are wet impregnated into g-C_3N_4 nanosheet support. PdNPs can serve as photocatalysts under visible-light irradiation, it is expected that the photocatalytic performances of g-C_3N_4 nanosheet can be further improved after loading of PdNPs. The loading weight percentages were changed from 0.2, 0.35, and 0.5% to examine the impact of Pd loading. By making the g-C_3N_4 photocatalyst into a 2D nanosheet structure, the inherent flaws can be somewhat overcome. Additionally, by adding noble metal nanoparticles, the photocatalytic performance existing can be greatly improved. A large amount of the sun's radiation is in the form of visible light (45%) and ultraviolet region (5%) and hence we have focused on the utilization of abundant visible light for biomass reforming. Our composite photocatalyst showed excellent visible light activity with H_2 generation rate of 1839.84μmol$g^{-1}h^{-1}$ within four hours of continuous irradiation and it is almost 27 times higher than undoped g-C_3N_4 nanosheets. For better understanding, three different Pd loading on g-C_3N_4 nanosheets were prepared, and glucose reforming efficiency was studied. In this pursuit of a better H_2 evolution visible light active photocatalyst, g-C_3N_4 nanosheet generated at various pyrolysis temperatures loaded with optimized Pd weight percentage is also explored.

Biography

Dr. Beena Mathew received her Ph.D. in Chemistry from Mahatma Gandhi University, Kerala, India. She was a JSPS Postdoctoral fellow at Kyushu University, Japan. Presently, she is a Senior Professor of Physical Chemistry at the School of Chemical Sciences and also Dean of the Faculty of Science at Mahatma Gandhi University. She is the former Director of the School of Chemical Sciences at Mahatma Gandhi University. Dr. Mathew supervised 40 research students and has 206 publications. The current research areas include green synthesis of nanoparticles and quantum dots, nanomaterials-based optical and electrochemical sensors for diverse applications, computational aspects of electrochemical and fluorescence sensing applications of nanomaterials, nano photocatalysts for wastewater remediation, metal nanoparticles doped photoactive supports for hydrogen generation through photocatalytic water splitting, and self-assembled supramolecular materials for various applications.

Single-nucleotide polymorphisms in MTHFR gene related to recurrent abortion

Yasin Kareem Amin[1,2]

[1]General Director of Medical Research Center, Hawler Medical University, Iraq
[2]General Director of Medico Legal Institute of Kurdistan, Iraq

Single-nucleotide polymorphisms are a type of genetic variation that may be utilized to investigate illness vulnerability. Recurrent abortion is linked to hereditary thrombophilias, which include various disorders such as the MTHFR thermolabile variation. No link is known between these two mutations and the risk of recurrent spontaneous abortion. It is unknown if pregnant women with these mutations are at risk of losing their baby. Thirty patients were referred to this prospective and experimental investigation with clinical results that included repeated spontaneous abortions. Peripheral blood samples were used to isolate total genomic DNA. PCR–restriction fragment length polymorphism method and Sanger sequencing technique were used to estimate the frequency of MTHFR gene polymorphisms in patients. The frequency of homozygous and heterozygous MTHFR polymorphisms were found in 80% and 20% among patients, respectively. Two samples with heterozygous MTHFR polymorphisms with recurrent abortion were followed and sequenced to know mutation type and location. Sanger sequencing results revealed that several frameshift mutations were seen, which includes (insertion, deletion and substations). This study highlighted some evidence that might play a role in the relationship between MTHFR polymorphisms and recurrent spontaneous abortion. Furthermore, we believe that anticoagulant medication for these individuals during pregnancy may result in a successful pregnancy.

Biography

Prof. Dr. Yasin Kareem Amin, a distinguished figure in embryology and *In Vitro* Fertilization (IVF), earned his Ph.D. in Embryology in 2009, showcasing a deep commitment to advancing knowledge in embryonic development. With an MSc in Anatomy and Histology in 2002, and a High Diploma in Forensic Anthropology from Bournemouth, UK, in 2005, Dr. Yasin has demonstrated expertise in diverse scientific domains. His medical journey began with an M.B.Ch.B degree from Mosul University College of Medicine in 1990, laying the foundation for his subsequent specialization in embryology and assisted reproductive technologies. As an IVF specialist, Prof. Dr. Yasin has made significant contributions to academic and scientific communities, playing a pivotal role in advancing reproductive medicine. His extensive educational background and practical experience highlight his dedication to the multifaceted aspects of medical and biological sciences.

Rotamerism, geometrical isomerism and intramolecular proton transfer in curcuminoids

Francis A. S. Chipem and **Sophy A. Shimray**

Department of Chemistry, Manipur University, India

Overexposure of human skins to UV radiation causes unfavorable effects such as photoaging, DNA mutation and generation of reactive oxygen species. To prevent such harmful effects, sunscreens are applied on skins for protection from UV radiation. Apart from aesthetically pleasing ingredients, the major component of sunscreens is a UV filter whose fundamental property is the dissemination of the absorbed UV radiation through intramolecular rearrangements. Currently, the commercially available UV filters are mineral sunscreens like zinc oxide or titanium dioxide or organic filters such as oxybenzone, homosalate and avobenzone. Curcuminoids, a group of naturally occurring compounds found in turmeric, have structural resemblance with avobenzone **(Chart 1)** in the centers of the molecules where diketo-enol tautomerism occurs followed by intramolecular proton transfer. The presentation discusses about our theoretical calculations employing density functional theory which shows possible rotamerism, geometrical isomerism and excited state intramolecular proton transfer (ESIPT) in the excited state in curcuminoids after absorption of UVA region (315-400 nm). These processes exhibit efficient dissipation of absorbed radiation in other forms of energy thus showing a potential application of curcuminoids as UVA filters. The calculations identify four geometrical isomerism as a result of rotation about C_2=C_3, C_8=C_9, and C_{11}=C_{12} double bonds leading to formation of eight different geometrical configurations. In addition, as many as 128 possible rotamers due to rotation about C_2-C_8, C_4-C_{11}, C_9-C_{10}, and C_{12}-C_{13} single bonds are identified which are in equilibrium both in the ground and first excited singlet states. Further, in configurations where there are six-membered cyclic intramolecular hydrogen bonded rings in the centre of the molecule, ESIPTs occur with small or no barrier in the intramolecular proton transfer reaction.

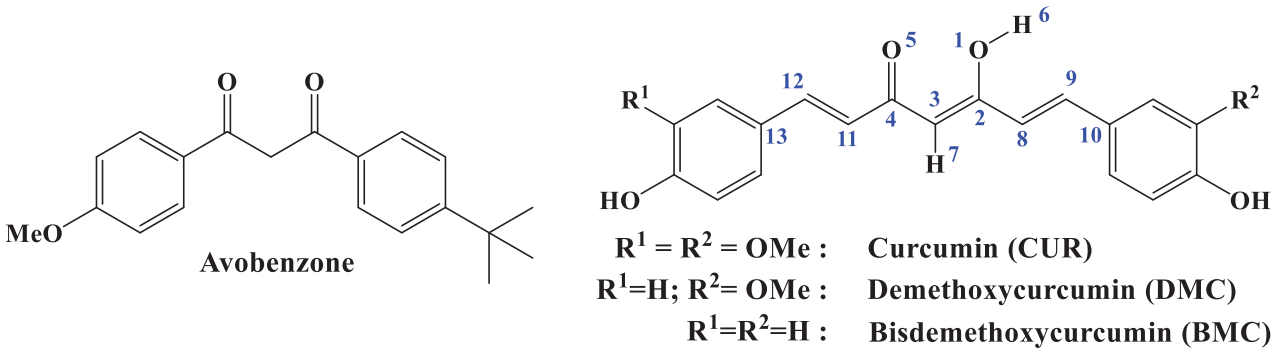

Chart 1. Structures of Avobenzone and Curcuminoids

Biography

Francis Chipem is currently working as Assistant Professor since 2013 in the Department of Chemistry, Manipur University, India. He received his master's degree in Chemistry from the Indian Institute of Technology Kanpur in 2007. He obtained his Doctor of Philosophy in 2013 from the Indian Institute of Technology Guwahati. His interests in research include photophysical study of bichromophoric organic molecules, catalysis and mechanism in organic reactions, and exploration of the applications of two-dimensional structures in energy storage.

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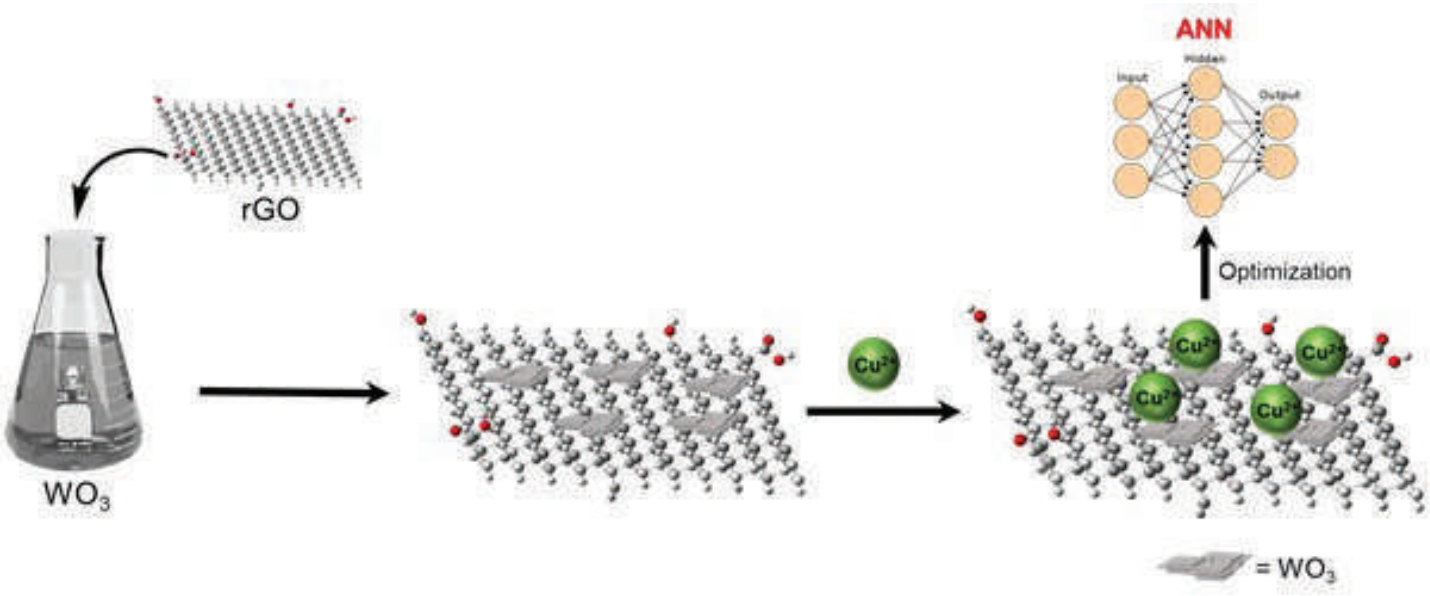
Insights into the adsorption mechanism of graphene oxide functionalized WO_3 nanocomposite for removal of Cu(II) ions from aqueous solutions: Kinetics, equilibrium, thermodynamics and artificial neural network modelling

B. Kavitha[1], K. Eswaran[2] and **S. Sivakumar[3]**

[1]Department of Chemistry, C.P.A. College, India
[2]School of Chemical Engineering, Yeungnam University, Republic of Korea
[3]Department of Computer Science, C.P.A. College, India

Industrial discharge-induced heavy metal contamination poses a significant environmental challenge. Reduced Graphene oxide (rGO), an emerging material, demonstrates exceptional performance in the realm of water treatment. The rGO modified WO_3 nanoadsorbents (rGO@WO_3) were synthesised and characterized by XRD, SEM, EDX, HR-TEM, FT-IR, XPS and BET analysis techniques. The rGO@WO_3 were used to selective removal of Cu(II) ions from aqueous solution was evaluated under different experimental parameters: pH, contact time, initial Cu(II) ions concentration, agitation speed, rGO@WO_3 dosage and temperature. The solution pH was highly influenced and rGO@WO_3 was worked well at pH 7. The maximum adsorption capacity for rGO@WO_3 was 48.53 mg/g. The prediction of Cu(II) adsorption were investigated via three-layered artificial neural network (ANN) model. The adsorption isotherm data of Cu(II) were well fitted to the Langmuir isotherm model and confirmed the monolayer coverage as described from the rGO@WO_3 morphology. The adsorption kinetic performance was rapid as the Cu(II) ions on rGO@WO_3 well with pseudo second order kinetic model equilibrated within 45 min. The interaction mechanism operates as follows: lone pair electrons in groups such as $C{=}O^-$, $C{-}O^-$, and $W{-}O^-$ coordinate towards Cu(II), fostering chemical interaction. The notable adsorption efficiency of rGO@WO_3 suggests promising applications in heavy metal remediation. The neural network architecture consisted of tangent sigmoid transfer function (tansig) at hidden layer with 10 hidden neurons, linear transfer function (purelin) at output layer and Lavenberg-Marquardt (LM) backpropagation training algorithm. The neural network model predicted values are found in close agreement with the batch experiment result with correlation coefficient (R) of 0.998 and mean squared error (MSE) 0.00852.



Biography

Dr. B. Kavitha

She received her B.Sc and M.Sc in chemistry (2009 & 2011) and obtained Ph.D. from Bharathiar University in 2018, supervised by Prof. Sarala Themabvani. She is currently working as an Assistant Professor of Chemistry at C.P.A College, Tamilnadu, India. Her research interests include photocatalysis, nanoadsorbents, artificial neural networks and environmental remediation.

Dr. K. Eswaran

He received his B.Sc. and M.Sc. degree in chemistry from Madurai Kamaraj University (2012 & 2015). He gained Ph.D. in chemistry from Kongju National University under guidance of Prof. Sanghyuk Park (2022). Then, he joined Yeungnam University, as an International Research Professor with Prof. Yong Rok Lee in 2022. His current research interests are the transition metal catalyzed C-H bond activation and annulation reactions.

Dr. S. Sivakumar

He earned his M.S. in Software Systems from Birla Institute of Technology and Science, Pilani, in 1996. He obtained his Ph.D. from Madurai Kamaraj University in 2010. Since 1989, he has been dedicated to academia, starting as a lecturer at C.P.A. College, Tamil Nadu, India. Currently serving as a Professor at C.PA. College, his research interests span various fields, including cloud computing, job scheduling, medical image reconstruction, soft computing, machine learning, Python, and material science.

Multitask learning for the segmentation of red blood cells in a sickle cell anemia diagnosis using efficient optimised efficient net model

Princy Matlani

Assistant Professor, Guru Ghasidas Vishwavidyalaya, India

An abnormal red blood cell called Sickle cell anemia (SCA) which causes blood vessel obstruction and even may death. This Sickle cell anemia is otherwise known as abnormal hemoglobin. In our body, the hemoglobin is used to passing oxygen all over the body through the blood vessels. The normal red blood cells are compact and flexible, so it is easy to move freely in small capillaries also and it is circular in shape. The reason for the pain to patients, decrease in oxygen level and dehydration is because of abnormal red blood cells in the human. Abnormal red blood cells are sickle in shape and they are stiff and angular causing them to become stuck in small capillaries. Therefore, the manual classification requires more time for the detection of RBC. So, to improve the classification accuracy and also to classify the erythrocytes into three classes, the novel optimized network model is introduced. Also, to fine-tune the hyper parameters and diminish the loss function of the network model the meta-heuristic strategy is jointly contributed with the deep learning model. As well as the over fitting issues are optimized by data augmentation schemes. In the experimental section, the efficacy of the proposed model is evaluated by analyzing essential performance metrics like accuracy, precision, recall, f-measure and dice similarity coefficients.

Biography

Dr. Princy Matlani (Orchid id: https://orcid.org/0000-0002 7421-8366) completed MTech. degree from the National Institute of Technology (NIT), Raipur, India, in 2013, and awarded PhD in Computer Vision in surveillance systems in year 2020. She is an active member of IEEE and Women in Engineering, IEEE. Presently, she is working as an Assistant Professor in Guru Ghasidas Vishwavidyalaya, Bilaspur, India (A central University). Her current research areas include image processing, medical image processing and computer vision based surveillance systems. She has published many research articles in reputed SCI journals and other WoS journals.

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Analysis of the mineralogical and chemical compositions of the laterization products of the parent rock of African major Bauxite deposits

Nafiu M. Zainudeen[1,2], Dennis K. Adotey[2,3], Andrew Nyamful[3,6], Latifatu Mohammed[4], Juliet Attah[3], Anita Asamoah[3], Benjamin K. Offei[5] and **Shiloh K. Osae[2]**

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[5]BNARI, Ghana Atomic Energy Commission, Ghana
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The production and export of Bauxite from Africa has been on the rise since its discovery there in the 1900s. Currently, the mining capacities of this ore in Africa are about a third of the World's total. The only economic challenge, however, is lack of siting of the processing plants that lead to final finished product; aluminium metal; seldom take place in Africa, resulting in loss of potential revenue from value chain of the product. The aim of this research is to review the mineralogical and geochemical properties of the known African Bauxite deposits which have been scientifically investigated to ascertain any existing trend for type of source rock and laterization products. Judging from obtained data, gibbsite is found to be the main aluminium hydroxide in all the deposits with slight occurrence of boehmite in 3 out of the 13 identified deposits, while goethite is the main oxyhydroxide of iron mineral. The highlight of the compiled results of the various investigations revealed the deposits have always been of diverse qualities relative to the World's standard regarding constituent elements and minerals. While the average percentage concentration of Al_2O_3 ranges between (43.73-61.25), that for Fe_2O_3 were between (1.55-34.25) and SiO_2 between (0.42-10.84). With evaluated silica moduli less than 8 for only two of the deposits (4.76 and 6.94), the rest have higher moduli ranging from (14.49-75.45). The higher percentage of Fe_2O_3 content (> 20%) in six out of the 13 deposits, allowed their grouping into three

categories: high alumina, ferruginous, and siliceous ores. Source rock of the deposits was determined through geochemical and petrographic considerations of laterisation products through evaluation of weathering indices: namely, Chemical Index of Alteration which were ranging between (97.16-99.98) and Ruxton ratio between (0.0133-0.2100); signifying intensive weathering process the parent rock underwent. Consequently, it was concluded that the source rocks of the laterization products are either anorthositic, argillite & dolerite, granulite & feldspathic gneiss, and mafic-basaltic andesite igneous.

Biography

Dr. Nafiu Mohammed Zainudeen is a Chemical Engineer by profession. He is a Research scientist with Institute of Scientific and Technological Information (INSTI); one of the 13 institutes of the Council for Scientific and Industrial Research (CSIR), Ghana. He is currently the lead Scientist at the Fluid Science Division of INSTI. His research interests have been from Renewable energy with emphasis on Biogas production, Fuel cell development and its operation and Separation process where ethanol-water mixtures are separated into fuel grade to power vehicles.

His bachelor's degree was from Middle East Technical University, Ankara Turkiye. He completed his master's programme from Kwame Nkrumah University of Science and Technology, Kumasi, Ghana, where he specialized in Separation processes.

His current field of interest is investigating the extraction techniques of Gallium from Bauxite. This research has been the main project for his just completed PhD programme in Nuclear & Environmental Protection at the University of Ghana, Legon.

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Subchronic toxicity study of herbal tea of Moringa stenopetala (Baker f.) Cudof. and Mentha spicata L. leaves formulation in Wistar albino rats

Abinet Admas[4], Abdu Hassen Musa[1], Asfaw Debella Hagos[2], Girmai Gebru Dimsu[1], Eyasu Makonnen Eshetu[3], Mesfin Asefa Tola[4], Abiy Abebe Gelagle[2] and **Boki Lengiso Tullu[5]**

[1]Department of Anatomy, School of Medicine, College of Health Sciences, Addis Ababa University, Ethiopia
[2]Traditional and Modern Medicine Research Directorate, Ethiopian Public Health Institute, Ethiopia
[3]Department of Pharmacology and Clinical Pharmacy, College of Health Sciences, Addis Ababa University, Ethiopia
[4]Department of Pathology, Saint Paul's Hospital Millennium Medical College, Ethiopia
[5]Directorate of National Reference Laboratory for Clinical Chemistry and Hematology, Ethiopian Public Health Institute, Ethiopia

Background: Moringa stenopetala (Baker f.) Cudof. and Mentha spicata L. are widely used in the traditional system of medicine for the treatment of diabetes, hypertension, digestive problems and various disorders. The leaves formulation of M. stenopetala and M. spicata herbal tea showed better antidiabetic and antihypertensive effects in rodent models. However, its long-term safety profile has not been investigated yet. Thus, this study investigated the subchronic (90 days) oral toxicity of the leaves formulation of M. stenopetala and M. spicata herbal tea in Wistar albino rats.

Methods: Four groups of rats (n = 10, with 5/sex/group) were randomly assigned into a control (vehicle) group and three test groups (559.36, 1118.72 and 2237.44 mg/kg, respectively). The three test groups received the herbal tea of M. stenopetala and M. spicata leaves blend daily for 90 days. The control group received distilled water. During the treatment period, clinical signs were observed daily, and food consumption and body weight changes of the rats were measured weekly. At the end of the experiment, macro-pathological, hematological and biochemical parameters were evaluated. Furthermore, histopathology of liver, kidney, heart, stomach and pancreas were examined.

Results: Subchronic oral administration of the herbal tea of M. stenopetala and M. spicata leaves blend did not result in death or significant toxicity signs in the treated group rats.

Moreover, the herbal tea caused no significant changes on body weight, food intake, organ weight, hematological and biochemical parameters in either sex. However, the serum AST, CK and LDH levels were significantly elevated in rats treated with 2237.44 mg/kg of herbal tea in both sexes. There was no significant alteration in the histology of organs, only minor lesions in the liver, kidney and pancreas were observed.

Conclusion: The study results indicate that the herbal tea of M. stenopetala and M. spicata leaves blend is relatively safe/low toxic to rats in subchronic exposure. However, further preclinical (chronic, teratogenic, reproductive and developmental toxicity) studies in animals are required in order to have sufficient safety and toxicity profiles for its use in humans.

Biography

Abinet Admas was born and raised in Addis Ababa, Ethiopia. After the completion of her higher education, she joined Hayat Medical School to complete her Doctorate degree. Then she won a scholarship to continue her residency in Pathology at Saint Paul's Hospital Millennium Medical College.

She has been working as a pathologist for the Ethiopian Federal Police Referral Hospital and in several private hospitals for the past four years. She has participated in several research projects, including the effects of traditional herbal leaves on internal organs and cervical cancer screening programs. She was also engaged in teaching undergraduate students and residents.

She is hard-working and always eager to learn new things and improve her skills. She has been awarded as 'best-practicing pathologist of the year 2022 G.C.' from Onco Pathology Diagnostic Center in Ethiopia.

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Protein folding problem: Enigma, paradox, solution

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[2]Biotechnology Department of the Lomonosov, Moscow State University, Russia
[3]Biology Department of the Lomonosov Moscow State University, Russia
[4]Center of Life Sciences, Skolkovo Institute of Science and Technology, Russia

The ability of protein chains to spontaneously form their spatial structures is a long-standing mystery in molecular biology. The mystery is how the protein chain can find its native, "working" structure without exhaustive enumeration of all possible conformations, which would take billions of years. This is the so-called "Levinthal's paradox." In this review, we discuss the key ideas and discoveries leading to the current understanding of protein folding, including the solution of the Levinthal's paradox. A special role here is played by the "all-or-none" phase transition occurring at protein folding and unfolding and by the point of thermodynamic (and kinetic) equilibrium between the "native" and the "unfolded" phases of the protein chain (where the theory obtains the simplest form). The modern theory provides an understanding of key features of protein folding and, in good agreement with experiments, it (i) outlines the chain length-dependent range of protein folding times, (ii) predicts the observed maximal size of "foldable" proteins and domains. Besides, it predicts the maximal size of proteins and domains that fold under solely thermodynamic (rather than kinetic) control. Complementarily, a theoretical analysis of the number of possible protein folding patterns, performed at the level of formation and assembly of secondary structures, correctly outlines the upper limit of protein folding times.

Biography

Alexei V. Finkelstein:

- Graduated with honors from the Moscow Phys.-Tech. (1970). Ph.D. (1976); D.Sc. (1991).
- Since 1970, member of the Laboratory of Protein Physics (then headed by Prof. O.B. Ptitsyn) at the Institute of Protein Research, Russian Academy of Sciences. Heads this Laboratory since 1999.
- Professor at the Moscow Lomonosov University since 1998. Soros Professor (2001).
- Author of ~300 papers, of a book "Protein Physics", published in Russian (7 editions), English (2 editions), Chinese (2 editions), and of a book "Physics of Protein Molecules" (in Russian).
- Citation index: 11000, Hirsch index: 50.
- Expertise: Protein physics; theory of protein structures, folding and design; structural transitions in proteins and amyloids; antifreeze proteins and ice nucleators, phase transitions; force fields; molecular biology; bioinformatics.
- Awards from FIRCA, INTAS, CASP, HHMI (3 times), NWO, etc.; State Prize of Russia in Science & Technology (1999).
- Elected to the Russian Academy of Sciences (2008).

Development of a new PET tracer [68Ga]68Ga-DOTA-ECL1i to non-invasively track fibrotic changes in myeloproliferative neoplasms based on C-C Chemokine receptor 2 detection

Silvia Migliari[1], Cecilia Carubbi[2], Anna Gagliardi[1], Maura Scarlattei[1], Giorgio Baldari[1], Marco Vitale[2], Elena Masselli[2] and **Livia Ruffini[1]**

[1]Nuclear Medicine Division (OU1), Azienda Ospedaliero-Universitaria di Parma, Italy
[2]Department of Medicine and Surgery (DiMeC), University of Parma, Italy

Myeloproliferative neoplasms (MPNs) are group of hematologic malignancies among which Myelofibrosis (MF) is the most aggressive [1]. Differential diagnosis of MF from other MPN subtypes is mandatory, due to prognostic relevance and need of timely therapeutic intervention. So far, only an invasive procedure such as bone marrow biopsy allows differential diagnosis of MF from other MPNs, Our research project proposes a new, non-invasive diagnostic algorithm to detect fibrotic stage in MPN based on the detection of hematopoietic progenitors (CD34+ cells) expressing the chemokine receptor CCR2, that we demonstrated being a unique feature of MF and not of healthy subjects and other MPNs [2-3], by the combination of PET imaging and peripheral blood flow cytometry (FCM).

To this aim, we developed and validated a targeted PET radioligand, 68Ga-DOTA-ECL1, able to detect CCR2+ cells [4] and validated FCM detection of CCR2+/CD34+ cells as diagnostic tool to differentiate diagnosis of MPN subtypes.

Methods: Radiosynthesis of 68Ga-DOTA-ECL1i was performed using a $^{68}Ge/^{68}Ga$ generator (GalliaPharm® Eckert & Ziegler) connected to an automated synthesis module (Scintomics GRP®). The radiopharmaceutical production was optimized scaling down the amount of DOTA-ECL1i from 50 to 10 µg of peptide precursor (50-40-30-20-10 µg).

Synthesis efficiency and release criteria were assessed according to *Ph. Eur.* for all the final products evaluating radiochemical yield (RY%), radiochemical purity (RCP% = 100%-colloids-ions), presence of free gallium (by Radio-UV-HPLC) and gallium colloids (by Radio-TLC), molar activity (Am), chemical purity, pH and LAL test.

Once the method was optimized, the process and the final product were validated with three consecutive syntheses whose stability was assessed over time.

The percentage of circulating CD34+/CCR2+ positive cells in different MPN subtypes was determined by flow cytometry Peripheral blood samples (3-5 mL in EDTA tubes) were processed with lyse & wash protocol. After labeling with antiCD45-FITC, antiCD34-PerCP-Cy5.5 and antiCCR2-PE, CD34+/CCR2+ cells were identified combining CD45 and CD34 staining with the analysis of lateral dispersion, or side scatter (SSC), and frontal dispersion, or forward scatter (FSC). % of CD34+/CCR2+ cells were obtained by plotting CD34-PerCP-Cy5.5 vs. CCR2-PE.

Results: Best results were yielded with 20 µg DOTA-ECL1i with optimal RY% (66.69%), RCP% (100%) and molar activity (45.41 GBq/µmol) (Table 1). The process validation (three batches produced on three different days) confirmed optimal RY% (mean value 64%) and molar activity (mean value 43.57 GBq/µmol). RCP% was 100% in all three batches (Fig. 1A-B) and the radiopharmaceutical resulted stable for at least 3 h after production, as shown by Radio-UVHPLC and Radio-TLC (Fig. 1C-D).

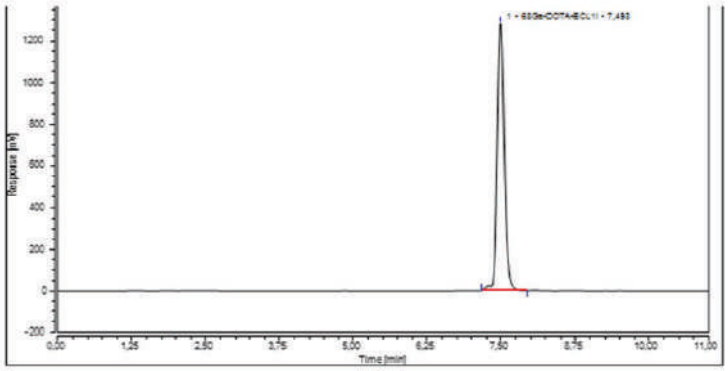
MF, pre-fibrotic form (prePMF, left panel) shows a higher percentage of circulating CD34+CCR2+ cells (18%) as compared to another MPN (essential trombocythemia, ET, 0.1%) (Fig. 1E). ROC curve of FCM analysis of CD34+CCR2+ cells in ET vs MF (pre-fibrotic form) demonstrates a very good diagnostic accuracy in discriminating the two disease subtypes ((AUC) of 0.8864 (95% CI: 0.7799–0.9928, P<0.0001) (Fig. 1F).

Next steps will be noninvasive tracking of CCR2+ cells by PET with 68Ga-DOTA-ECL1 in Gata-1low mouse model of MF and assessing the feasibility of 68Ga-DOTA-ECL1i PET imaging in patients to discriminate MF from other MPN subtypes.

Conclusions: We hypothesize that this new non-invasive diagnostic strategy will be extremely helpful to guide and assist the clinicians in phenotyping MPN, to support hemopathologist in controversial differential diagnosis and to detect extramedullary sited involvement by tracking CCR2+CD34+ cells in the sites of extramedullary hematopoiesis.

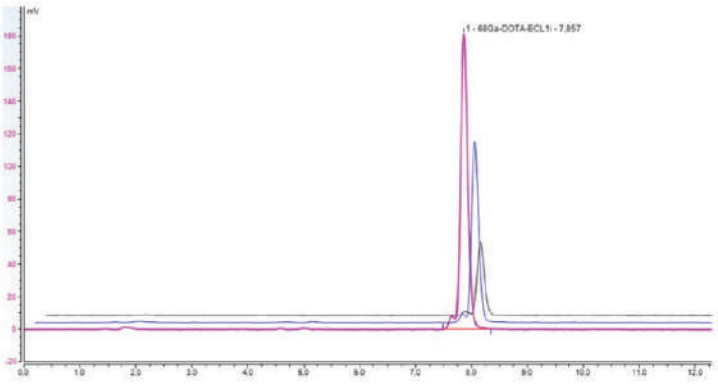
Peptide (DOTA-ECL1i, ug)	50 (250 µL, 0.038 µmol)	40 (200 µL, 0.031 µmol)	30 (150 µL, 0.023 µmol)	20 (100 µL, 0.015 µmol)	10 (50 µL, 0.0076 µmol)
Radiochemical purity (Radio-UV-HPLC)	100%	100%	100%	100%	100%
Radiochemical purity (Radio-TLC)	100%	100%	100%	100%	100%
pH	7	7	7	7	7
Radiochemical yield (n.d.c.)	55.90%	54.03%	62.45%	66.69%	53.21%
Volume	10	10	10	10	2–10 mL
Color	Colorless	Colorless	Colorless	Colorless	Colorless
Molar activity	15.026 GBq/µmol	16.51 GBq/µmol	30.34 GBq/µmol	45.41 GBq/µmol	71.51 GBq/µmol

Table 1. Summary data of [68Ga]68Ga-DOTA-ECL1 QCs according to the peptide scale down (10–50 µg, n = 3)

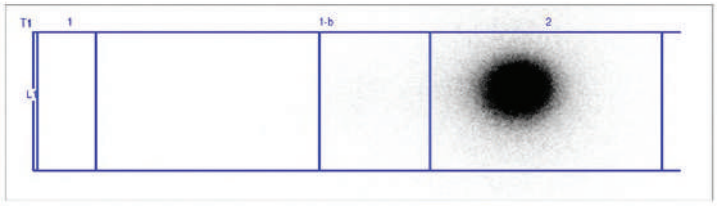


(A)

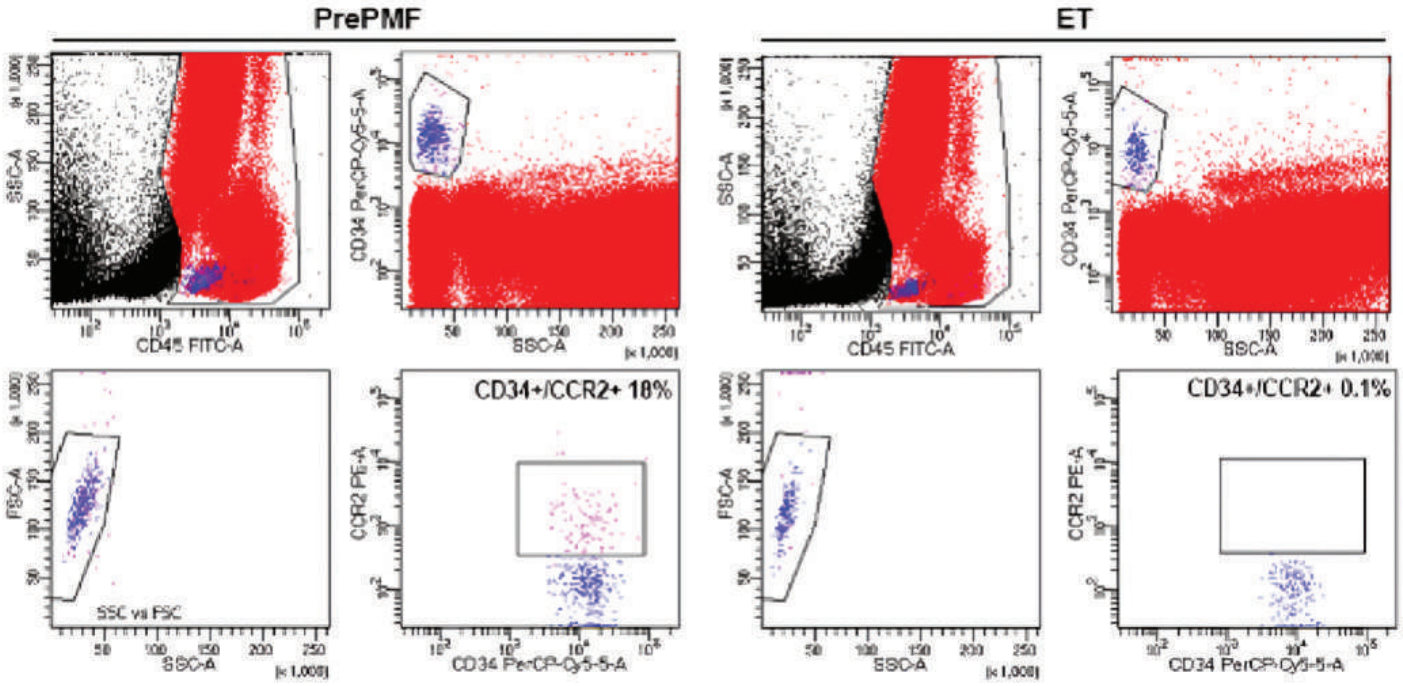
(B)

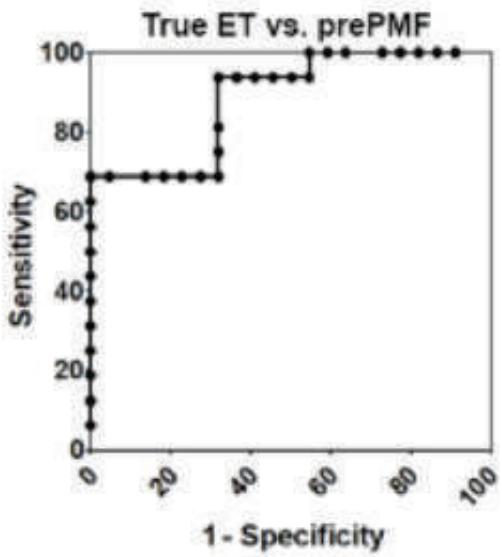


(C)



(D)





ROC CURVE	
AUC	0.8864
95% C.I.	0.7799-0.9928
P value	<0.0001
Sensitivity (%)	68.8
Specificity (%)	100.0
PPV (%)	100.0
NPV (%)	81.0

Figure 1. (A) Radio-UVHPLC chromatogram of [68Ga]68Ga-DOTA-ECL1; (B) Radio-TLC chromatogram of [68Ga]68Ga-DOTA-ECL1; (C) Stability of [68Ga]68Ga-DOTA-ECL1 (pink dash: 1 h, blue dash: 2 h, black dash: 3 h); (D) Radio-TLC chromatogram of [68Ga]68Ga-DOTA-ECL1 over 3 h. (E) Flow cytometric (FCM) detection of CD34+/CCR2+ cells in peripheral blood sample of a representative MF, prefibrotic form (left) and essential thrombocythemia (right). (F) Diagnostic accuracy of FCM detection of CD34+/CCR2+ cells; Area under the curve (AUC), confidential interval (CI), P value, cut-off value, sensitivity, specificity, positive predictive value (PPV) and negative predictive value (NPV) are reported.

Next steps will be noninvasive tracking of CCR2+ cells by PET with 68Ga-DOTA-ECL1 in Gata-1low mouse model of MF and assessing the feasibility of 68Ga-DOTA-ECL1i PET imaging in patients to discriminate MF from other MPN subtypes.

Conclusions: We hypothesize that this new non-invasive diagnostic strategy will be extremely helpful to guide and assist the clinicians in phenotyping MPN, to support hemopathologist in controversial differential diagnosis and to detect extramedullary sited involvement by tracking CCR2+CD34+ cells in the sites of extramedullary hematopoiesis.

Biography

Silvia Migliari was born on February 14th, 1987, in Reggio Emilia, Italy.

She has a master degree in Chemical and Pharmaceutical Technologies, cum laude (2007-2011) and a specialization in Hospital Pharmacy, cum laude (2013-2017), both at the University of Parma, Italy.

She is the Qualified Person of the Radiopharmacy Laboratory at the Nuclear Medicine Division of Azienda Ospedaliero-Universitaria di Parma (IT) where she worked since 2012.

She have a solid expertise in managing production and quality controls of radioligands for clinical applications, as well as in development, validation and IMPD editing of new tracers in the research context (since 2012 up today >1650 SPECT preparations; since 2015 up today >1800 PET preparations), with the final aim to obtain new translational imaging biomarkers targeting specific disease pathways (PMID:36729317; 35056858; 35190517; 33687908; 34374683; 33754194;32990551; 32567505; 33642752; 33525300; 33525262; 31580314; 30333459; 29520394). She involved in many multidisciplinary research projects.

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Solubility of fluorite in concentrated electrolyte solutions at elevated temperatures: Implications to nuclear waste-form development and rare earth element (REE) extraction

Yongliang Xiong[1], Yifeng Wang[1], Guangping Xu[2] and **Vanessa Mercado[1]**

[1]Department of Nuclear Waste Disposal Research & Analysis, Sandia National Laboratories (SNL), USA
[2]Department of Geochemistry, Sandia National Laboratories (SNL), USA

Fluorite with a chemical formula of CaF_2 is versatile wasteforms that can accommodate a wide range of nuclear wastes. The nuclear wastes that fluorite-type wasteforms can accommodate include fluoride molten salt wastes, actinides, fission products such as Cs-135, Cs-137 and Sr-90, etc. The molten alkali fluoride salts [e.g., (Li, Na, K)F] have utility in the applications to the next generation of nuclear reactors. The fluorite wasteforms are a strong candidate for immobilization of such alkali fluoride salts contaminated by fission products. Geologically, fluorite is an important host-phase for rare earth elements (REE) in various geological formations. For instance, fluorite can occur in greisen pockets of granites, in skarns, and in hydrothermal veins.

In this work, we have conducted solubility measurements on fluorite at 25°C and 60°C. Based on our experimental results and solubility data from the literature, we establish a thermodynamic model describing solubilities of fluorite in various media to high ionic strengths and to elevated temperatures. In the modelling, we use the Pitzer equations and the Specific ion Interaction Theory (SIT) for activity coefficient calculations. Based on our model, the stability of fluorite wasteforms in terms of its solubility under various conditions can be predicted. Similarly, the leaching efficiency under various conditions for REE sources hosted by fluorite can also be predicted.

Sandia National Laboratories is a multi-mission laboratory operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. This research is funded by the SFWST programs from the Office of Nuclear Energy (NE), and a project from the Office of Fossil Fuel Energy (FE), U.S. Department of Energy (US DOE). SAND2024-01168A.

Biography

Dr. Yongliang Xiong is a geochemist. He joined Sandia National Laboratories in 2002. Prior to joining Sandia, he was a Research Associate at Rutgers University at New Brunswick, New Jersey. He has authored or co-authored more than 80 peer-reviewed publications, with extensive expertise in solution chemistry/geochemistry of actinides, aluminium, boron, lead, platinum group elements (PGE), rare earth elements (REE), rhenium (an analogue to radiogenic technetium), selenium, silica, and thallium. Dr. Yifeng Wang is a geochemist with more than 110 publications. He has extensive experience in nuclear waste disposal. Dr. Guangping Xu is a geochemist. He joined Sandia National Laboratories in 2017. Prior to Sandia, he worked at Schlumberger – Doll Research in Cambridge, MA as a research scientist and Colorado State University in Fort Collins, CO as a research associate. Vanessa Mercado is a year-around student intern at Sandia National Laboratories.

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Water quality evaluation and impact of nitrogen contamination

Sharadha Sambasivan[1], Kathryn M. Gutleber[1], Aayush Pande[2,4] and Shreyas Prakash[3,4]

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[4]College of Agricultural and Life Sciences, Cornell University, USA

This project focuses on the chemical analysis of various available sources of water such as municipal water supply at home and at the local water bodies (streams, lakes, river, bay) in Long Island, NY. A comparison study of water quality from chemical analysis-lab data with publicly available Suffolk County Water Authority (SCWA) data was conducted. The water quality degradation due to human activities (cesspools, fertilization, pesticides, chemical/industrial wastes) vs natural process such as in relation to Nitrogen-cycle was further studied. The increased nitrogen loading in water is of particular interest since Long Island's drinking water is drawn from a sole-source aquifer, and the primary means of waste disposal is through individual cesspools/septic tanks, particularly in Suffolk County, the easternmost county on Long Island, NY. The water quality is evaluated based on the levels of contaminants, pH and dissolved oxygen. The total nitrogen level was determined from measuring the nitrates, nitrites and ammonium content, and phosphates level were measured too. The testing of lead and heavy metals on a qualitative level (presence or absence) will also be included in the study. Preliminary data suggests that in a few zip codes in Suffolk County nitrogen content as nitrates in local water streams are higher than allowable by Environmental Protection Agency. To continue to prevent and limit the lead and nitrate content in our groundwater, and in turn, our drinking water, Long Island's residents must be educated about the harmful effects of lead and nitrate, and how they enter our drinking water in the first place. Additional studies by students included an examination of a new septic system currently being piloted in Suffolk County which reduces Nitrogen loading.

Biography

Dr. Sharadha Sambasivan is a Professor of Chemistry at Suffolk County Community College, NY actively engaged in undergraduate chemical education research. She served as Principal Investigator on a NASA –CCI grant and collaborator on NIH and NSF grants to develop Introduction to Research Methods course. Through this course she has mentored over 18 students to pursue science research. She serves as chair of chemistry assessment committee (2012-2017 and 2023-2028) for college, member of Middle States Accreditation team, Curriculum development committees and Equity and Inclusion Council. She has created innovations in cooperative learning, blended/flipped learning pedagogies in undergraduate chemistry courses. Her research at Brookhaven National Laboratory involved x-ray characterization of biomaterials, polymers, catalysts relevant in industry. She was fellow of Department of Energy's Visiting faculty program characterizing functionalized graphene compounds utilizing spectroscopic, magnetic and electrical methodologies. In 2019 she was the recipient of SUNY Chancellor's award of Excellence in Faculty Service.

Conformational changes of human stratum corneum lipids by effect of cyclic and linear siloxanes

Krystyna Mojsiewicz-Pieńkowska and **Dagmara Bazar**

Department of Physical Chemistry, Faculty of Pharmacy, Medical University of Gdańsk, Poland

Introduction: Siloxanes (silicones) are widely used in various dermatological and personal care products as well as cosmetics, both for children and adults. Their unique properties (biocompatibility, chemical stability) and numerous advantages (like smoothing, moisturizing and softening the skin), more than 50% cosmetics contain at least one type of silicone. However, the essential issue is that the increasing number of scientific reports indicate toxicological impacts due to directly contact these compounds with cells or tissues. Some siloxanes have been recognized as, for example, disrupting the endocrine, immune, neuron or metabolic systems. Our last innovative studies also proved that siloxanes can impact on human skin and weaken its barrier function. Hence, this research is focus on investigating the mechanism and one of the reasons of weaken skin barrier, as well as the safety estimation of using skin products contain linear or cyclic siloxanes.

Aim of Study: The aim of studies was identification the interactions siloxanes with *stratum corneum* lipids on microscopic and molecular levels and estimation of their conformational changes.

Methods: The research methodology was based on the official guidelines for the study of dermal absorption of xenobiotics, published by the Organization for Economic Cooperation and Development (OECD) and the World Health Organization (WHO). The study was conducted comparatively, using a test group (ex vivo human skin after siloxane application; 6 different compounds were selected) and a control group (ex vivo skin without siloxanes application), using the Transdermal Diffusion Cell System, Hanson Research Corporation, USA. The estimation of the interaction's siloxanes with stratum corneum lipids were conducted:

a) on the microscopic level - by using fluorescence microscopy

b) on the molecular levels - by using attenuated total reflection Fourier-transform infrared spectroscopy (ATR-FTIR) technique.

Results and Conclusion: The microscopic images receiving after stained by hydrophilic dyes (fluoresceine FLU and sulphorhodamine B - SRB) outlined that the structure of the stratum corneum has been disrupted after all siloxanes application. Part of corneocytes were deformed and lost the natural hexagonal or pentagonal shape. Also, the black spaces were visible what confirmed the destruction of this skin layer which is a crucial for barrier function.

An important observation was to prove irreversible destruction of the lipid matrix surrounding corneocytes, what explained the reason for the loss of correct corneocyte structure. The probable mechanism was according with diffusion siloxanes to skin and lipids extraction (e.g. ceramides, fatty acids and cholesterol) by the lipophilic siloxanes.

Using ATR-FTIR technique, we confirmed that siloxanes can interact with stratum corneum lipids although the strength of the interaction depends on the type of siloxane. Both band shifts (with wavenumbers approx. 2920, 2852, 1745, 1464, 1402 [cm^{-1}]) and changes in their surface areas were identified. This allowed to confirm the conformational changes in lamellar and lateral organization, focusing attention on both the observation of orthorhombic, hexagonal, liquid crystal (fluid) phases, as well as the change in the conformation of lipid chains from trans to gauche.

Acknowledgment: This study was financial supported by the Polish National Science Centre, OPUS Program, Grant no. DEC-2018/31/B/NZ7/02801.

Biography

Krystyna Mojsiewicz-Pieńkowska is an Assistant Professor at the Department of Physical Chemistry of Faculty of Pharmacy at the Medical University of Gdansk, Poland.

Her principal research interests are focused on: estimation human skin barrier; safety assessment of transdermal diffusion; interaction the substances with skin lipids and proteins; development the innovation analytical methods for pharmaceutical studies with validation protocols.

Her research also focuses on the: development of topical pharmaceutical products including adhesive skin patches; analysis of various matrices (human skin layers, adhesive skin patches, drugs, cosmetics); examination of the physicochemical properties of amorphous and crystalline drugs to improve the pharmacokinetic properties and bioavailability.

Montmorillonite-based chitosan nanocomposites as sustainable slow-release green fertilizers

P. Siriphannon[1,2], S. Rukchonlatee[1,2], S. Rungkron[2], S. Soetsom[2] and S. Sukyee[2]

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In this study, we present a novel approach for the efficient synthesis of montmorillonite-chitosan nanocomposites as slow-release green fertilizers, denoted as MMT/xCS-yKNO_3-zTPP. The nanocomposites were prepared through a simple stepwise incipient wetness impregnation method. The initial compositions were varied, i.e. KNO_3 to MMT ranging from 10-30 wt%, chitosan to MMT ranging from 2.5-10 wt%, and TPP: chitosan weight ratios ranging from 0:5, 1:5, and 3:5. The process began with the impregnation of montmorillonite (MMT) with a mixture solution of protonated chitosan (CS) and potassium nitrate (KNO_3). This resulted in the capillary penetration of protonated chitosan and KNO_3 into the basal spacing of MMT. Subsequently, the impregnation with sodium tripolyphosphate (TPP) solution facilitated the crosslinking of protonated chitosan. The resulting nanocomposites comprised a crosslinked chitosan matrix embedded with KNO_3, which was intercalated within the basal spacing of MMT and partially covered its surface. The impregnated potassium and nitrate ions effectively interacted with the charged MMT sheets and protonated chitosan, becoming entrapped within the crosslinked chitosan network, filling the confined spacing of the MMT structure. Therefore, these nanocomposites exhibited unique properties that synergistically slowed the release of potassium and nitrate plant nutrients. In simulated cultivation experiments using RD43 rice seedlings, the application of MMT/xCS-yKNO_3-zTPP nanocomposites resulted in notable increases in seedling height and root growth. Overall, our research presents an innovative and sustainable approach to slow-release green fertilizers, utilizing montmorillonite-chitosan nanocomposites. These nanocomposites have the potential to enhance agricultural practices, promote crop growth, and serve as eco-friendly solutions for long-term nutrient supply in plant cultivation.

Biography

Associate Professor Punnama Siriphannon obtained her Ph.D. in Inorganic Materials from Japan's Tokyo Institute of Technology in 2000, marking a pivotal moment in her academic journey. Her research primarily centers on nanomaterials, with a focus on montmorillonite-based nanocomposites, chitosan-based nanocomposites, and metal oxide nanoparticles. Dr. Siriphannon's expertise and dedication have garnered recognition, including a prestigious nomination for the L'Oréal-UNESCO for Women in Science Fellowship in 2012. She is highly regarded as a prominent figure in the field of nanomaterials, making significant contributions to both research and education. Beyond her research and teaching roles, Dr. Siriphannon actively participates in public outreach and science education. As a dynamic speaker, she has delivered numerous enlightening talks and presentations on nanomaterials to diverse audiences, including students, educators, and the general public. Her efforts bridge the gap between cutting-edge scientific discoveries and the wider community, fostering greater understanding and appreciation for the world of nanomaterials.

Graphene assisted optical tweezers and its applications

Yuquan Zhang

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The excellent physical properties of graphene have greatly improved the performance of optoelectronic devices and brought important technological advances to optical research and its applications. Here, graphene is introduced to the field of optical-tweezer technology and demonstrate a new graphene-based opto-thermoelectric tweezer. This technology not only reduces the incident light energy required by two orders of magnitude (compared with traditional optical tweezers), it also brings new advantages such as a much broader working bandwidth and a larger working area compared to those of widely researched gold-film-based opto-thermoelectric tweezers. This graphene-assisted optical tweezers demonstrate enormous application potential in trapping or concentration of cells and biomolecules as well as to microfluidics and biosensors.

Label-free Raman spectroscopic detection of cellular elements is an important technique for biological science applications; however, the implementation of proactive intracellular detection remains a challenge. Here, we employ the graphene-based thermoelectric optical tweezers system in intracellular Raman spectral detection on-a-chip applications. Because of the excellent photothermal conversion effect of the graphene substrate, a potent thermoelectric effect is generated to not only strengthen the trap for biological cells, but also accelerate metallic nanoparticles to permeate into these cells for intracellular Raman enhancement. An *in situ* intracellular Raman spectrum is thus acquired that offers the opportunity to distinguish the intracellular elements. This work provides a promising approach for cytobiology research and is expected to enable exciting new applications in the detection of complex intracellular life processes.

Biography

Yuquan Zhang, received his PhD in optical engineering from Nankai University, China, in 2015. Currently, he is an associate professor in the Nanophotonics Research Center of Shenzhen University. His research interests include singular optical field modulation, optical tweezers, surface/tip-enhanced Raman spectroscopy, and super resolution imaging. Recently, his research has focused on nano-optical trapping and nonlinear effects in optical traps.

Polyol-based extraction: A green approach to extract bioactive compounds for cosmetic and tropical products

Nuntawat Khat-udomkiri[1] and **Hla Myo**[2]

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[2]College of Public Health Sciences, Chulalongkorn University, Thailand

For several decades, organic solvents have been extensively employed in cosmetic and pharmaceutical applications to extract bioactive compounds from plant materials and agricultural wastes. This is primarily due to their widespread availability and cost-effectiveness. However, these solvents must be eliminated from the extract prior to being incorporated into the formulation due to their potential skin toxicity. Methods for solvent elimination will be expensive, time-consuming, and energy-intensive. In order to address this issue, there has been significant research development focused on polyols as a potential substitute solvent for the extraction of bioactive compounds. This talk aims to highlight our new research findings regarding the efficacy of polyols in the extraction process of phenolic compounds from various agricultural wastes and plant materials, such as coffee pulp, *Camellia sinensis* flowers, and *Rhus chinensis* Mill. leaves. Furthermore, the extract derived from polyols showed higher efficacy in terms of both *in vitro* and cellular antioxidant activities when compared to their ethanolic extract. In addition, some polyol-based extracts had greater cell viability in skin fibroblasts than ethanolic extracts. Moreover, the utilization of polyols in conjunction with unconventional extraction methods has the potential to enhance the presence of bioactive molecules and their antioxidant ability. Thus, polyol-based extractions can be regarded as environmentally friendly alternatives for extracting bioactive substances and are suitable for implementation in the cosmetic and pharmaceutical industries.

Biography

Dr. Nuntawat Khat-udomkiri earned his B. Sc. (Hons) in Cosmetic Science from the Mae Fah Luang University, Chiang Rai, Thailand in 2014 and Ph. D. in Pharmacy from Chiang mai University, Chiang Mai, Thailand in 2020. After receiving his Ph.D., he was hired as a full-time lecturer in the School of Cosmetic Science, Mae Fah Luang University. His current research interests focus on the optimization of bioactive compounds extraction from agricultural wastes and plant materials using nonconventional extraction techniques with polyols as alternative solvents for cosmetic applications. Furthermore, he is also interested in cell-based assays for safety and efficacy in cosmetic applications, nanodelivery systems in cosmetics, and novel cosmetic formulations.

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Synthesis and molecular structure studies of Aluminium (III) complexes with β-ketoiminate and ethanolamine ligands

Leonardo Santoni and **Caroline E. Knapp**

University College London (UCL), UK

Aluminium, a cost-effective and abundant metal known for its high conductivity, holds promise for use in printed electronic wiring. However, its susceptibility to oxidation has limited its industrial application. Research on utilizing aluminium-based complexes for metal conversion has been constrained by handling challenges arising from their reactivity to moisture and air. Recent advancements in precursor design, incorporating stable bidentate ligands, demonstrate significant progress in overcoming handling challenges, showcasing significant progress in this field.[1] We present the design, synthesis, and potential applications of β-ketoiminate and ethanolamine aluminium precursors, whilst retaining a reasonable shelf-life. Compounds of the type $[AlL_3]$ have been synthesised from trimethylamine alane (TMAA) with the β-ketoiminate ligands.[2] The reaction of $LiAlH_4$ with the β-ketoiminate resulted in three classes of compounds: $[AlL_3]$, Li-cages[3], and chelated aluminates.[4,5] Additionally, using TMAA and ethanolamine formed $[L_3(L'Al)_3Al]$. To date, these reactions have been applied to L = Me-acnac, tBu-acnac, Ph-acnac, Mes-acnac and Dipp-acnac. Moreover, for the ethanolamines, the reactions have been applied to L' and L" = N,N- $(Me)_2$ ethanolamine and N,N- $(Et)_2$ ethanolamine (Figure 1). These reactions have been explored with different ratios between the starting materials, revealing some exciting results related to the structures and decomposition profiles. Ultimately, the obtained products were applied across diverse methodologies to facilitate the deposition of the metal, aiming to identify the most efficient approach.

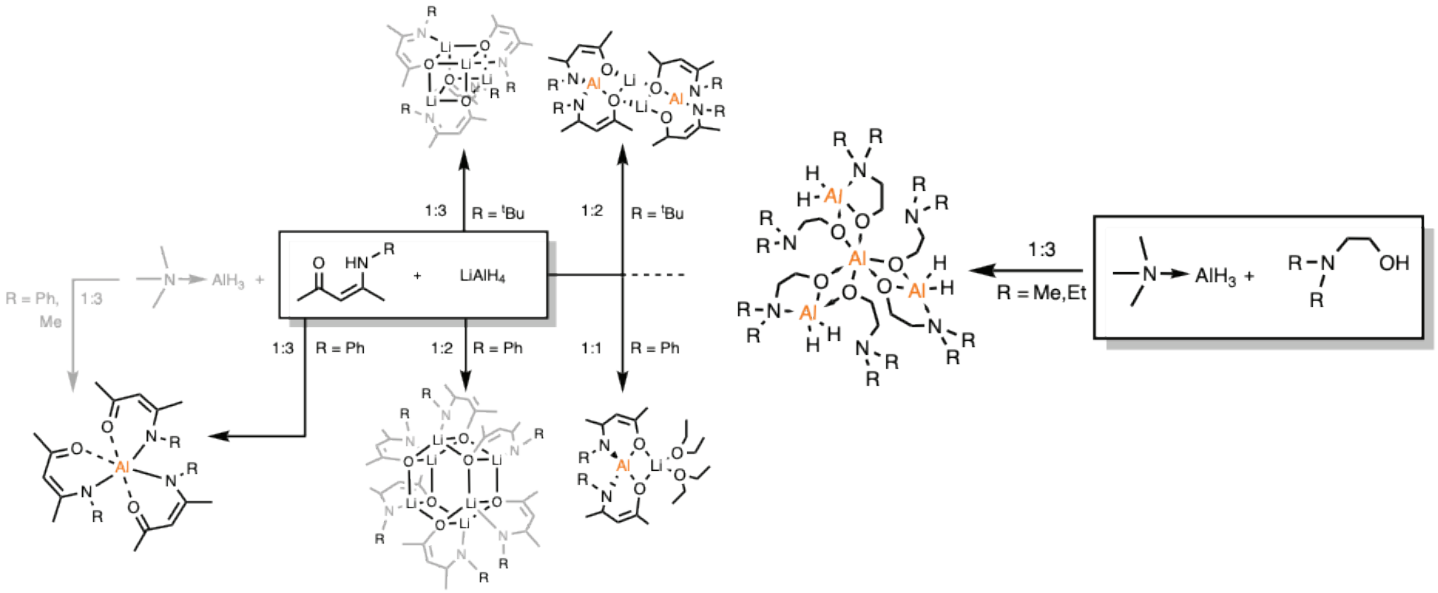

Figure 1. Reactions scheme: β-ketoiminate Ligands (Left) vs. Ethanolamine Ligands (Right) with Aluminium Sources.

Biography

Leonardo Santoni, currently pursuing his PhD at University College London (UCL). His research focuses on synthesizing aluminium precursors for functional materials within Caroline E. Knapp's Research Group. He earned his master's degree in chemistry from Alma Mater Studiorum, specializing in organic, analytical, physical, and coordination chemistry.

His professional journey includes conducting GiSANS and Reflectivity analyses at ISIS Neutron and muon source and Institute Laue-Langevin. He mentored Master's students, served as an NMR analysis consultant for EpiValence LTD and Sava Technologies, and taught chemistry at UCL. He undertaken research internships at the University of Copenhagen and CNR, ISOF in Bologna, working on projects ranging from organic chemistry to the synthesis of composite materials.

He is a member of prestigious societies like the Royal Society of Chemistry and the Society of Chemical Industry.

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Advanced insights into phenylpropene biosynthesis in *Ocimum basilicum* L.: The role of vermicompost form, dose, and application method

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In this study, we explored the impact of vermicompost on phenylpropanoid metabolism in basil's Peltate glandular trichomes (PGTs). We tested 0, 10%, and 25% doses of solid and tea forms of vermicompost on the methylchavicol chemotype of basil. Gene expression *(PAL, 4CL, EGS, EOMT, CVOMT)* and phenylpropene accumulation (eugenol, chavicol, methyleugenol, methylchavicol) were analyzed post-treatment. Solid vermicompost (SV) at 10% and 25% doses significantly reduced *EOMT* and *CVOMT* expression and decreased methyleugenol and methylchavicol levels by up to 76% and 52%, respectively. Conversely, 10% vermicompost tea (VT) significantly increased chavicol and methyleugenol levels by 243% and 613%, respectively, and upregulated *EOMT* and *CVOMT* expression. A 25% VT dose also increased eugenol and methylchavicol levels while down regulating the same genes. Our findings indicate that VT modulates phenylpropene accumulation through gene regulation, enhancing basil's aroma and antimicrobial properties. This study underscores the utility of PGTs in plant secondary metabolism research and the potential of vermicompost in phytoremediation.

Biography

Dr. İlker Türkay is an academician and biologist with a focus on the biochemistry of medicinal and aromatic plants, phenylpropanoid metabolism, and plant systematics. Holding a Ph.D. in Biochemistry and an M.Sc. in Plant Taxonomy, he currently serves as a Lecturer at Kırşehir Ahi Evran University. His prior roles include Practicing Expert at the Faculty of Agriculture and Medical Representative for international pharmaceutical firms. Dr. Türkay's unique blend of academic and commercial experience equips him with a nuanced understanding of both scientific research and its real-world applications. Passionate about educating the next generation of scientists, he is committed to contributing to academic and scientific communities through research and collaboration.

Electrical conductivity, microstructures, chemical compositions, and systematic multivariable models to evaluate the effect of waste slag smelting (pyrometallurgical) on the compressive strength of concrete

Ahmed Salih Mohammed[1,2], Nzar Shakr Piro[3] and **Samir M. Hamad[4]**

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[3]Civil Engineering Department, Faculty of Engineering, Soran University, Iraq
[4]Scientific Research Centre, Soran University, Iraq

This study explores the application of steel slag, a by-product of pyrometallurgical steel production, as a substitute for fine and coarse aggregates in concrete. The research aims to contribute to resource conservation and optimize landfill space. The chemical composition of steel slag, characterized by significant silica, aluminum oxide, calcium oxide, and other elements, varies based on the steelmaking process. The study collected, analyzed, and modeled a dataset of 338 entries to identify factors influencing the compressive strength of concrete with steel slag substitution. Key parameters included water/cement ratio, steel slag content, fine aggregate content, and coarse aggregate content. Additionally, 134 data points on electrical conductivity were collected to assess its impact and correlation with compressive strength. Utilizing various models, including linear regression, nonlinear regression, artificial neural network (ANN), full quadratic model (FQ), and M5P-tree model, the study predicted compressive strength, with the ANN model employed for electrical conductivity. The results indicated enhanced compressive strength with increased steel slag content. Statistical analyses demonstrated the superior predictive accuracy of the ANN model, providing valuable insights into optimizing concrete properties through steel slag integration. The research underscores the efficacy of the ANN model in achieving precise predictions of compressive strength and emphasizes its potential in advancing concrete technology.

Biography

Dr. Ahmed Salih Mohammed is an accomplished Assistant Professor with affiliations at the University of Sulaimani and the American University of Iraq, Sulaimani. He completed his Ph.D. and Postdoctoral Research at the University of Houston, Texas, USA. Driven by a continuous pursuit of knowledge, he earned his M.Sc. in Civil Engineering in 2003 and his BSc. in Building and Construction Engineering in 2000.

With expertise spanning Nanotechnology, Geotechnics Engineering, Drilling Engineering, and more, Dr. Mohammed has made significant contributions to the field. His impressive research impact is reflected in a citation count of 7000+, an h-index of 52, and authoring 245 publications. Recognized as the top-ranked Iraqi researcher in construction and building materials from 2021-2023, he has also served as a reviewer for over 30 international journals and held editorial roles in five journals with notable impact factors.

Acknowledged as one of the World's Top 2% Scientists by Stanford University in 2021, 2022, and 2023, Dr. Ahmed Salih Mohammed stands as a leading figure in the global academic and research community. His multifaceted career continues to inspire and contribute significantly to the advancement of knowledge in Civil Engineering.

Tumor cell adhesion and metastasis signaling: Contribution of endothelium nitric oxide

Fabiola Sánchez[1,2], Pamela Ehrenfeld[1,2], Gaynor Aguilar[1] and Tania Koning[1]

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Metastasis is the main cause of death in cancer patients. The endothelium plays a key role in metastasis allowing the adhesion and extravasation of tumor cells. Nitric oxide (NO) is a key modulator of the endothelial function and we have demonstrated that the stimulation of endothelial cells with secreted factors from breast tumor cells induces S-nitrosylation (the modification by NO of cysteine residues in proteins) of endothelial proteins leading to destabilization of the endothelial barrier which may contribute to transmigration of breast tumor cells and metastasis. The first step in the extravasation process leading to metastasis is the attachment of cancer cells to the endothelium. This step shares similarities with leukocyte adhesion to the endothelium, and it is plausible that it may also share some regulatory elements. We report that the stimulation of endothelial cells with cytokines present in the serum of cancer patients (TNF-α, IL-8) or with secreted factors from breast tumor cells activates the S-nitrosylation pathway and increases leukocyte adhesion *in vitro* and *in vivo*. The stimulation also increases the cell surface availability of the adhesion proteins VCAM-1 and ICAM-1 in endothelial cells in a NO and S-nitrosylation dependent way. We identified PKCz and VCAM-1 as S-nitrosylated targets during this process. Inhibition of NO signaling and S-nitrosylation blocks the transmigration of tumor cells through endothelial monolayers and the development of metastasis in a murine model of breast cancer. We propose that S-nitrosylation in the endothelium activates pathways that enhance surface localization of adhesion proteins to promote binding of tumor cells and extravasation leading to metastasis.

Biography

Dr. Fabiola Sánchez studied Biochemistry at the Austral University of Chile. She obtained her Doctorate in Biological Sciences, mentioning Cellular and Molecular Biology at the Pontifical Catholic University of Chile. She later completed her Postdoctorate in Vascular Biology at the University of Medicine and Dentistry of New Jersey, United States.

CdO nanostructures as acid-base bifunctional heterogeneous catalysts for making Coumarin-3- Carboxylic Acids at room temperature

R. Kaur and **S. K. Mandal**

Indian Institute of Science Education and Research Mohali, India

In this work, cadmium oxide (CdO) nanostructures were synthesized by calcining three different cadmium-based coordination polymers (CPs) at 600°C. For the synthesis of these nanostructures, **CP-1, CP-2**, and **CP-3** were used as single source precursor material. Detailed formula for **CP-1**: $\{[Cd_2(bpta)_2(adc)_2]\cdot 2H_2O\}_n$; **CP-2**: $\{Cd_2(bpea)_2(adc)_2\}_n$; **CP-3**: $\{Cd_2(bpma)_2(adc)_2\}n$; (here, bpta = N,N'-bis(pyridyl *t*-butyl) amine, bpea = N,N'-bis(pyridylethyl) amine, bpma = N,N'-bis(pyridylmethyl) amine and adc = acetylene dicarboxylate). Then temperature-dependent study was also conducted by varying the temperature from 600°C to 700°C, and 800°C for three of the CPs yielding corresponding product in good yield. The synthesized material was analysed by energy dispersive X-ray spectroscopy (EDX), powder X-ray diffraction (PXRD), high-resolution transmission electron microscopy (HRTEM) for its crystallinity and purity investigation. Surface morphological studies were confirmed by field-emission scanning electron microscopy (FESEM), which indicated the presence of spherical, octahedron and icosahedron shaped particles at 600°C to 700°C, and 800°C, respectively. The optical properties were examined by solid-state UV-vis diffuse reflectance spectra and band gap values in the range of 1.7-2.0 eV were calculated using Tauc plot. Exploring the dual properties of CdO nanostructures, as an example, **CdO_3a** was used to synthesize Coumarin-3-carboxylic acid synthesis at ambient conditions in the presence of methanol solvent for 1 h, giving 100% conversion. The catalytic efficiency of **CdO_3a** has been evaluated by performing recyclability test for minimum four cycles and found to be easily recoverable, and reusable without any loss in its activity. The phase stability, after being used in the catalysis has also been confirmed.

Biography

Rupinder Kaur was born in Punjab, India. She has received her five-year integrated BS-MS degree in 2018 from Sri Guru Granth Sahib World University, Fatehgarh Sahib, Punjab. She is also awarded with a Senior Research fellowship from University Grants Commission for her entire Ph.D. program. Currently she is continuing her Ph.D. degree from Indian Institute of Science Education and Research, Mohali under the supervision of Prof. Sanjay Mandal. Her

main research work focuses on synthesis of diverse semiconductor materials and metal- organic frameworks, and their application. She has also extended her work to synthesize nanoparticles@MOFs composites and to utilize them for various Lewis Acid catalyzed organic transformation reactions. She has research publications from some of her work that she has carried out until now in her Ph.D. program.

Composition and characterisation of ancient lime mortar of 12th century temple, Alandi, India

Sarvesh Singh[1], P. D Sabale[2] and **Manager Singh[3]**

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[2]Deccan College Deemed University, India
[3]Dr. Balasaheb Ambedkar Marathwada University, India

The cementing lime mortars used in the construction of 12th century A.D Gopal Krishna temple at Western India Alandi were investigated for its mineralogical, chemical and compositional characteristics. The investigative studies were performed using particle size studies, XRF, XRD, FTIR, SEM-EDX and thermal analysis of the mortar. Though the monument is situated in Sahyadri range of Deccan basaltic trap, the mortar is marked by mixing of aggregates rich in hydrated oxides of alumina and iron. Further studies revealed natural formation of laterite caping on basaltic hillock that preferentially weathered and sediments deposited along the river basin sourced as aggregates in mortar preparation. The lime rich binder has mainly inclusion of sub-angular to sub-rounded coarse grain lateritic aggregates. The clay impurities have reduced the purity of lime as observed through thermal analysis. The data will help prepare a compatible mortar for restoration.

Biography

Sarvesh Singh is Chemist / Assistant General Manager at the Reserve Bank of India Archives, Pune, Maharashtra, INDIA 411 016. He worked for HINDALCO Ind. Ltd. as an Analyst during 1998 to 2003. He has more than 20 years' experience in the field of conservation and preservation of cultural heritage. He holds PhD. in Chemistry, MBA in Finance, MA in History and Diploma in Heritage Sites Management and Scientific Conservation, Archaeology and Certificate in Archival Preservation and Practices, Records Management, Preservation of Archival Photographs, Managing Plans and Drawings, Preserving Microfilm etc. He was the recipient of fellowship to work at the Metropolitan Museum of Art, New York, USA. He is visiting faculty at Deccan College Pune for the Conservation of Cultural property. He has authored around 21 papers, published in various international and national journals on various subject. He attended and presented papers in in various international and national conferences.

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Calcium element quantification model using a portable X-ray fluorescence unit

Claudio Hernán González-Rojas[1], Cristián Castro-Rodriguez[1], Sebastián Gutiérrez-Vivanco[2] and **Esteban Vargas-Vera[1]**

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[2]Archaeometric Analysis and Research Laboratory (LAIA), High Research Institute, Universidad de Tarapacá, Chile

The methodology for heavy metal analysis is mainly based on the use of liquid phase techniques such as AAS and ICP-Mass. Their advantages are: high precision, low cost and low detection limits. Except for the time required for digestion, which ranges from one to two days.

The concurrence of another technique, X-ray fluorescence, made possible the qualitative determination of several metals of the Periodic Table as the two previous ones, except that the analysis is done in solid phase. This could mean a reduction in the total evaluation time. But another difficulty arises, the conversion of the number of emission counts to units suitable for comparison, either as % w/w or as mg/kg and the availability of appropriate solid-state standards.

This is why this analysis methodology was proposed: using the effective quantification of the element Calcium in ideal soil samples, with a portable X-ray Fluorescence (pXRF) equipment. The protocol began by preparing an ideal matrix using an increasing mass, of Calcium and Sodium Nitrate as binder. In this sample the fluorescent emission line of the element Calcium was calibrated using a standard reference material 1400 bone ash.

The validation of ideal samples of the element Calcium using the XRF technique with respect to AAS as an experimental standard, using linear correlation methods, allowed us to appreciate that both approaches remain above the standard curve provided by AAS, with a value of 1.68. Which means that the tendency to evaluate Calcium samples by XRF are overestimated with respect to the curve provided by AAS. Since the last correlation coefficient is very close to 1.0 and its statistical inference equation is precisely known, the authors of this work propose to apply quantification protocol to real sediment samples.

Biography

Claudio González is Chilean has got a PhD in Science from the University of Chile. He got Post Doctoral position in Molecular Electronics and Biomass from the same University. He is Full Professor at the Universidad de Tarapacá. He is founder of the Systems Modeling Laboratory of the Universidad de Tarapacá.

He has published in Materials Physicochemistry, Materials Engineering, Molecular Photophysics, Organometallic Synthesis and Atmospheric Sciences. Referee for the journals Atmospheric Pollution and Aerosol and Air Quality Research. He is developing research on mathematical and statistical models of air pollution. He has also worked in modeling using EPA codes such as Screen3©, ScreenView© and other open codes such as Rstudio©, OpenAir©, ALOHA© and HYSPLIT©. Member of the Thesis reviewer: Universidad de Chile, Universidad de Antioquia Colombia and Universidad Católica de la Santísima Concepción.

Environmental Consultant in Minera Pampa Camarones S.A., Somarco Ltda., and Compañía Minera Los Pelambres.

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Regulatory role of LexA in modulating photosynthetic redox poise and cadmium stress tolerance in the cyanobacterium, *Anabaena* sp. PCC7120

Yogesh Mishra[1], Akanksha Srivastava[1], Arvind Kumar[2], Subhankar Biswas[1], Vaibhav Srivastava[3] and **Hema Rajaram[2,4]**

[1]Department of Botany, Centre of Advanced Study in Botany, Banaras Hindu University, India
[2]Molecular Biology Division, Bhabha Atomic Research Centre, India
[3]Division of Glycoscience, Department of Chemistry, School of Engineering Sciences in Chemistry, Biotechnology and Health, Royal Institute of Technology (KTH), AlbaNova University Centre, Sweden
[4]Homi Bhabha National Institute, India

Strategies developed by organisms to overcome disruption in redox poise of photosynthetic electron transport chain (pETC) are important for its survival under abiotic stress. The process needs to be tightly regulated for optimal functioning. While the redox poising processes are well known in cyanobacteria, understanding of their regulatory network is lacking. Since LexA is one of the known global regulators of stress response in the cyanobacterium *Anabaena* sp. PCC7120, its role in pETC redox poising was investigated using cadmium (Cd) as an abiotic stressor to disrupt photosynthesis. Assessment of the photosynthetic responses of recombinant *Anabaena* strains, An*lexA*$^+$ (LexA-overexpressing) and AnpAM (vector control), under unstressed and Cd-stressed conditions using transmission electron microscopy (TEM) and chlorophyll a fluorescence, indicated that some pETC redox poising responses, including PSII photodamage, energy dissipation, PSI photoprotection, and NDH-mediated cyclic electron flow were decreased in An*lexA*$^+$ under unstressed conditions. Disturbance in pETC redox poise during Cd stress observed in *Anabaena* was accentuated upon overexpression of LexA. The decreased photodamage of PSII and increased photoinhibition of PSI in An*lexA*$^+$ in the presence or absence of Cd stress, correlated well with the changes in pETC complexes observed in blue native (BN)-PAGE and the regulation of over 70 of the 90 pETC component genes by LexA demonstrated through transcript, electromobility shift assay (EMSA), and bioinformatics studies. In a nutshell, LexA has been identified as one of the regulators involved in the streamlining of pETC redox poising responses under normal growth and during abiotic stress through transcriptional regulation of some of the redox-controlled pETC component genes.

Biography

Yogesh Mishra did his PhD from Banaras Hindu University in 2008. During his PhD research he had examined the effect of heat and UV-B stress on a filamentous cyanobacterium *Anabaena doliolum* at molecular level. After that he moved to Umea Plant Science Centre Umea, Sweden and joined the group of Prof. Stefan Jansson. During his more than five years of stay at Umea he has not only published articles in reputed journals but also, he had gained expertise higher plants molecular biology. To strengthen his expertise in the area of abiotic stress and hormone signaling, he joined the group of Prof. Koncz at Max Planck Institute for Plant Breeding Research (MPIPZ), Cologne, Germany as a post–doctoral researcher. He retuned back to India in 2014 as a group leader and currently trying to unravel the molecular mechanism of abiotic stress tolerance and signaling in cyanobacteria and plants using interdisciplinary approaches.

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Green practices implementation for environmental sustainability by five-star hotels in Kampala, Uganda

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Hotels and hotel business chains are known to be some of the biggest contributors of global pollution. In order to mitigate this, implementation of green practices is vital if not very essential. This study focused on implementation of green practices by five-star hotels found in Kampala district, Uganda, and specifically exploring the benefits achieved and effects encountered by the management of the hotels as a result of implementing green practices. An exploratory research design was employed to collect the required data from 197 employees of the five-star hotels. Data was collected using the semi-structured questionnaire and an interview guide. The study revealed energy conservation, waste management, and environmental purchasing with their respective Coefficient of Variances of 12.6, 14.5 and 17.2, as some of the green practices implemented by the hotels. The implementation of the green practices culminated into increased profits, competitive advantage, saved on the costs of the materials used and retained some customers. It is recommended that there should be continuous awareness and strengthening of training of the employees about green practices' implementation, together with government involvement in all matters concerning enforcement of green practices, all aimed for environmental sustainability.

Biography

Alex Barakagira (PhD) is affiliated to Kyambogo University, Kampala, Uganda. He has a PhD in Environmental Geography from Nelson Mandela University, South Africa. He is a lecturer at the Department of Environmental Science, Faculty of Science. He has a teaching experience of seventeen years and a senior researcher for five years at the University setting. His area of expertise includes Environmental Sciences; Climate Change; Public Health; Medicinal Plants and Essential Oils; Environmental Remote Sensing and GIS. He has published a number of articles and book chapters in both national and international peer reviewed journals. In addition, he has presented some scientific research papers at both regional and international conferences. He is also a participant in a number of scientific research collaborations with some regional and international Universities from Kenya, Ethiopia, Egypt, Nigeria, South Africa and Austria.

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Poly(amido amine) functionalized graphene oxide for enhancing properties of a polysulfone ultrafiltration membrane: Effect of Poly(amido amine) generation

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[2]Department of Chemical Engineering, Qatar University, Qatar
[3]Department of Civil and Architectural Engineering, Qatar University, Qatar

To meet the growing demand of water and to ensure sustainable growth of society, wastewater treatment and re use has gained prominence over the last century. Ultrafiltration is a low pressure driven membrane-based wastewater treatment technology that can be used to remove heavy metal, dye, oil, complex organics, pharmaceuticals and other pollutants from wastewater. However, polymeric ultrafiltration membranes used for wastewater treatment suffer from low flux, excessive fouling and low pollutant rejection rate due to the hydrophobic nature of the polymers. In order to enhance the hydrophilicity of the polymeric membranes, doping of polymeric membranes with hydrophilic functional groups containing nanocomposites has been suggested. Poly(amido amine) or PAMAM are nano-polymers which are radially symmetric 3-D molecules containing an amine or ethylenediamine core and are terminated by large number of amine molecules. The number of terminal amine groups depends on the generation of PAMAM and with each generation, the number of terminal PAMAM groups increases exponentially. The presence of high concentration of amine groups on the surface of the PAMAM makes them suitable for polymeric membrane applications. In this study, different generations of GO-PAMAM nanocomposites were prepared and incorporated in the polysulfone membrane matrix. The effect of PAMAM generation on the morphology and performance of the ultrafiltration membrane was studied. By cross sectional FE-SEM analysis, formation of finger-like voids in membrane matrix was confirmed in the modified membranes. While using generation 2 PAMAM, pure water permeation flux showed 10 times higher flux than the pristine polysulfone membrane. The membrane also showed more than 99% BSA rejection along with 20% improvement in flux recovery rate.

Biography

Ahmed Toky Yasir is a PhD candidate at the department of Chemical Engineering at Qatar University. His doctoral dissertation delves into the intricate synthesis of nanocomposites adorned with hydrophilic functional groups. This innovative approach forms the foundation for the creation of mixed matrix membranes, demonstrating a pioneering use in the treatment of produced water. The study not only emphasizes the synthesis process but also underscores the practical application of these nanocomposites, showcasing their efficacy in addressing environmental challenges associated with produced water treatment. Apart from the membrane process, his research interest also includes electrocoagulation, membrane bio reactors, dielectrophoretic coalescence and process modeling. He has published more than 10 peer reviewed articles in reputed journals during his PhD.

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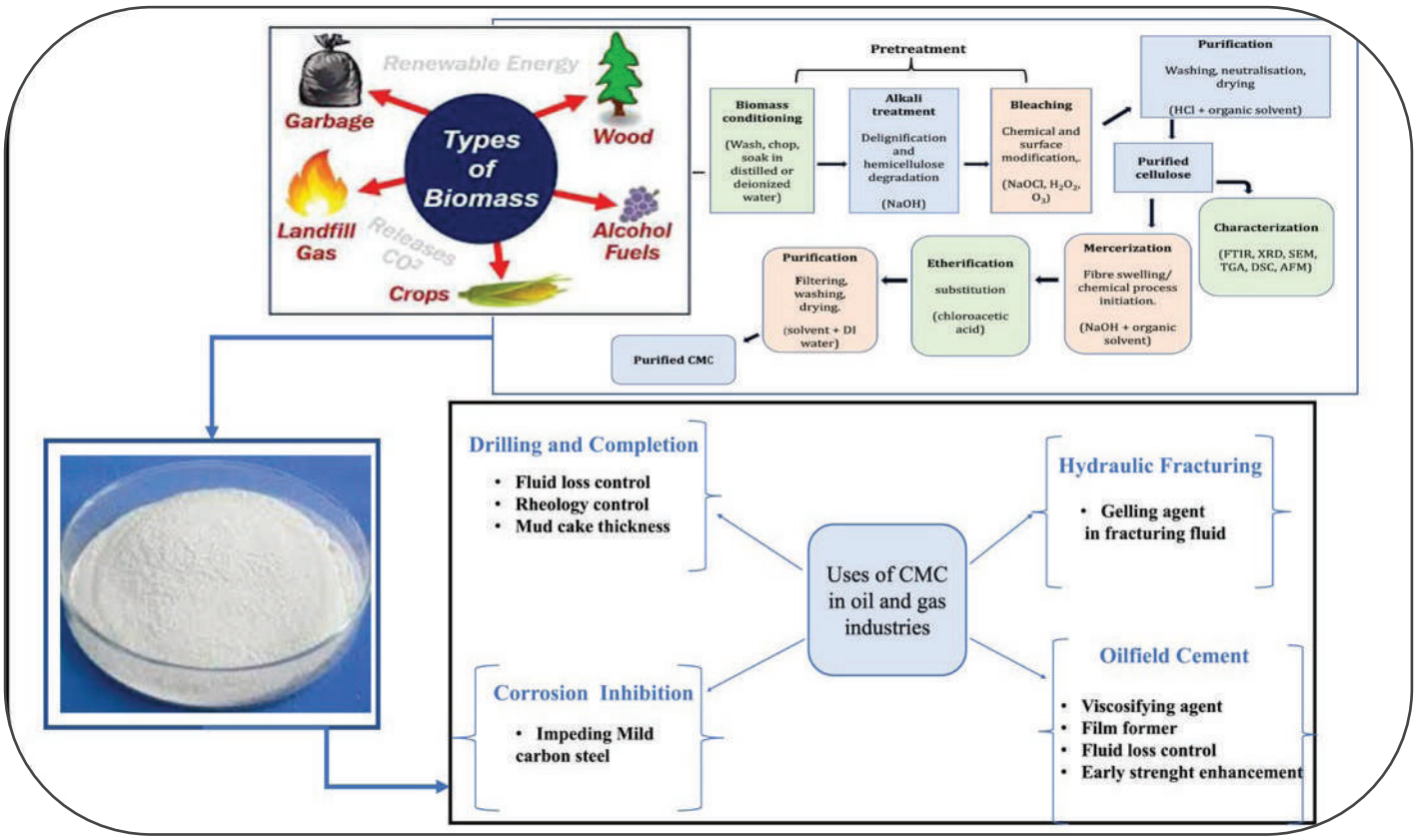
Carboxymethyl cellulose for oil and gas field operations

Hauwa A. Rasheed[1], Adekunle Adeleke[1], Petrus Nzerem[1], Olusegun Ajayi[2], Peter Ikubanni[3] and **Asmau M. Yahya[1]**

[1]Nile University of Nigeria, Nigeria
[2]Ahmadu Bello University, Nigeria
[3]Landmark University, Nigeria

Carboxymethyl Cellulose (CMC) is one of the most promising cellulose derivatives and the most widely used in the drilling sector. Owing to its multifunctionality, facile, inexpensive, raw material abundance, availability, compatibility, distinctive surface property and many other disparate aspects, it is now widely used in many fields for a variety of applications, including the oil and gas industry. CMC is used as a component in oilfield chemicals for applications including cementing, hydraulic fracturing, corrosion inhibition, and drilling and completion. Researchers are choosing and finding CMC precursor materials more appealing due to their availability and flexibility. Even though the sources of CMC were limited in the early stages of its development, numerous researchers or studies over the past few years have shown many of their alternatives. This work seeks to present a concise overview of its synthesis, the many opportunities for its use in the oilfield sector, and some of the difficulties associated with its application.



Biography

Hauwa holds a BSc in Chemistry from Bayero University, Kano and an MSc in Oil and Gas Chemistry from University of Aberdeen, UK. Hauwa is now a PhD student in Department of Industrial Chemistry, Nile University of Nigeria. She is currently working on “Synthesis and Optimization of Carboxymethyl cellulose from Agricultural wastes for use in oil and gas field operations”.

Monocyte HLADR and Immune Dysregulation Index as biomarkers for covid-19 severity and mortality

Namrata P Awasthi

Dr. Ram Manohar Lohia Institute of Medical Sciences, India

Background: Immune dysregulation in COVID-19 is the major causal factor associated with disease progression and mortality. Role of monocyte HLA-DR (mHLA-DR), neutrophil CD64 (nCD64) and Immune dysregulation index (IDI) were studied in COVID-19 patients for assessing severity and outcome. Results were compared with other laboratory parameters.

Methods: Antibody bound per cell for mHLA-DR, nCD64 and IDI were measured in 100 COVID-19 patients by flow cytometry within 12 h of hospital admission. Thirty healthy controls (HC) were included. Clinical and laboratory parameters like C - reactive protein (CRP), Procalcitonin (PCT), Absolute Lymphocyte count (ALC), Absolute Neutrophil count (ANC) and Neutrophil to Lymphocyte ratio (NLR) were recorded. Patients were followed up until recovery with discharge or death.

Results: Parameters from 54 mild (MCOV-19), 46 severe (SCOV-19) and 30 HC were analysed. mHLA-DR revealed significant and graded down regulation in MCOV-19 and SCOV-19 as compared to HC whereas IDI was lowest in HC with increasing values in MCOV-19 and SCOV-19. For diagnostic discrimination of MCOV-19 and SCOV-19, IDI revealed highest AUC (0.99). All three immune parameters revealed significant difference between survivors (n = 78) and non-survivors (n = 22). mHLA-DR < 7010 and IDI > 12 had significant association with mortality. Four best performing parameters to identify patients with SCOV-19 at higher risk of mortality were IDI, NLR, ALC and PCT.

Conclusion: mHLA-DR and IDI, in addition to NLR and ALC at admission and during hospital stay can be utilized for patient triaging, monitoring, early intervention, and mortality prediction. IDI reported for the first time in this study, appears most promising. Immune monitoring of 'in hospital' cases may provide optimized treatment options.

Biography

- Prof. Namrata P Awasthi has established Hematology Laboratory services for the tertiary care teaching institute which offers under graduate, post graduate and post-doctoral certification courses in sub specialties of Pathology.
- She did her MBBS in 2001, MD Pathology in 2006, Senior Residency in Lab Hematology in 2009.

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The problem of relation between excess and absolute adsorption: Rigorous results

Eduard S. Jakubov[1] and **Timur S. Jakubov**[2]

[1]A.N. Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Russia
[2]Retired. Formerly Professor, Swinburne University of Technology, Australia

The main content of the Gibbs science of adsorption is the development of a rigorous thermodynamics of two-dimensional excesses. The most important fundamental disadvantage of the adsorption excess method is the inevitable impossibility of comparing the results of the Gibbs thermodynamic calculation with the results of any real physical experiment. The point is that such an experiment involves all molecules near the interface, not only "excess" molecules. So, because of the fact that the primary experimental quantity in the study of adsorption from solutions is the excess adsorption isotherm, then the above-mentioned problem can be formulated as the problem of determining absolute adsorption from excess adsorption data. Usually, in most scientific works, this problem is solved by introducing some physical models that are based on different assumptions about the structure and properties of the interfacial boundary. In our work an attempt is made to solve the problem as rigorously as possible without involving any assumptions ю So far it has been known that the excess adsorption isotherm has one obvious special point: the maximum value of adsorption. In our work it is shown that there is another remarkable point, which is related to the limiting (absolute) value of adsorption. Knowledge of this second special point allows us to find the dependence of the concentration of the adsorption phase on the concentration of the bulk phase in an explicit form, while remaining within the framework of the data on the excess adsorption isotherm. The key new element in the proposed approach is a method to find this point on the excess adsorption isotherm where the rate of concentration growth of the predominantly adsorbing component reaches its mean value in adsorbed phase. The accuracy of predicted functions for absolute adsorption is within the accuracy of the original experimental data for excess adsorption isotherms.

Biography

Eduard S. Yakubov was born in February 1940 in Tbilisi, Georgia. After graduating from school in 1958, he entered the Mendeleev Institute of Chemical Technology in Moscow and graduated in 1963 obtaining the engineer's diploma in Chemical Engineering. In 1972-1976 he received a second education at the Moscow Institute of Electronics and Mathematics (MIEM), specializing in Applied Mathematics. He completed his Ph.D. in 2001, the title of his thesis was “Properties of adsorption solutions in zeolite NaX”. From 2002 to 2021 he was a visiting lecturer at the MIEM, where he taught courses in physical chemistry and statistical thermodynamics. On 28 May 2012 he was awarded the academic title of Associate Professor. Since 1978 to the present, he has been a researcher at the Laboratory of Physical-Chemical Bases of Chromatography and Chromatography-Mass Spectrometry of the Institute of Physical Chemistry and Electrochemistry of the Russian Academy of Sciences.

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In quest of small molecules as dengue NS2B-NS3 protease inhibitor using *in-silico* molecular docking

D. M. Nahar[1], P. B. Mohite[1], S. J. Tauro[1] and **M. A. Kanyalkar[2]**

[1]St. John Institute of Pharmacy and Research, India
[2]Principal K. M. Kundnani College of Pharmacy, India

Objective: To address the escalating threat of Dengue virus (DENV) and the absence of effective vaccines or antiviral medications, this study aims to design potential lead molecules targeting the NS2B-NS3 protease, a critical non-structural protein in DENV. The primary goal is to identify promising candidates through computer-aided drug design (CADD) and synthesize potential protease inhibitor possessing anti-dengue activity.

Scope: The study involves designing and analyzing about eight hundred compounds, including derivatives based on diverse scaffolds like cinnamic acid, chalcone, chalcone-cinnamic acid hybrids, substituted benzimidazole, and 2-amino-4-substituted thiazole. Emphasis is placed on assessing binding interactions with the NS2B-NS3 protease through molecular docking, along with cytotoxicity and *in-vitro* inhibitory activity evaluation.

Methodology: The research involves the utilization of CADD techniques to design compounds based on phytoconstituents and Nitazoxanide. Molecular docking is conducted using NS2B-NS3 protease structures (PDB ID: 2FOM) to analyze binding interactions, including H-bonding, hydrophobic, and ionic interactions, along with determining binding energy. Selected compounds are further synthesized, and their cytotoxicity and *in vitro* anti-dengue activity are evaluated.

Results: The designed molecules from 2-aminothiazole, cinnamic acid, chalcone, and their hybrids, as well as benzimidazole derivatives, exhibit varying degrees of inhibitory activity against the NS2B-NS3 protease. Selected compounds are synthesized and showed promising results in *in-vitro* anti-dengue activity. All designed molecules exhibit a significant reduction in viral titer and demonstrate non-cytotoxicity. Among the molecules, 4-phenylthiazol-2-amine (T1), 2-(4-tert-butylphenyl)-1H-benzo[d]imidazole (I5), and (2-(4-tert-butylphenyl)-1H-benzo[d]imidazol-1-yl) (phenyl) methanone (D3) emerge as particularly promising. These

compounds exhibit good protease inhibitory activity in the sub-micromolar range (IC_{50} = 5.5µM, 5.2µM, & 8.04µM, respectively), indicating robust antiviral potency.

Conclusion: This study contributes to the ongoing search for effective anti-dengue medicines by proposing potential lead molecules targeting the NS2B-NS3 protease. The diverse set of designed compounds, their molecular interactions, and the observed inhibitory activities offer valuable insights for further exploration and development of anti-dengue therapeutics.

Biography

Deepali Mahir Nahar, serving as an Assistant Professor in Pharmaceutical Chemistry at St. John Institute of Pharmacy and Research, affiliated with the University of Mumbai. She completed her M Pharmacy and have 13 years of teaching experience, guiding eight M Pharmacy students. Pursuing a PhD at the University of Mumbai, her focus is on "Development of Antiviral agents using Structure Aided Drug Design, Synthesis, and Evaluation." Her research interests include Synthetic Chemistry, Computer-Aided Drug Design, Microwave-assisted Drug Synthesis, and Analytical Method Development, emphasizing the synthesis and evaluation of novel pharmacologically active entities and antimicrobial agents. She has presented posters and papers at national and international conferences, and she hold life memberships in Indian Society for Technical Education (ISTE) and Indian Pharmaceutical Association (IPA), along with registration with the Maharashtra State Pharmacy Council of India.

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How can ice emerge at 0°c and what do ice-binding proteins do?

Alexei V. Finkelstein[1,2,3], Bogdan S. Melnik[1,2] and **Sergiy O. Garbuzynskiy[1]**

[1]Institute of Protein Research of the Russian Academy of Sciences, Russia
[2]Biotechnology Department of the Lomonosov, Moscow State University, Russia
[3]Biology Department of the Lomonosov Moscow State University, Russia

An examination of the freezing kinetics shows that (i) at small negative temperatures, the ice formation in bulk water takes enormous time and, therefore, can occur neither in lakes nor bodies; (ii) ice nucleation at small negative temperatures requires some ice-bonding surfaces, but (iii) even then, ice formation can typically occur at temperatures of about -10°C. However, some “ice-nucleating” surface can initiate the ice formation at virtually zero temperatures. The task of antifreeze proteins is not, as it was commonly believed, to bind to ice crystals that have been already formed and stop their growth, but to bind to various “ice-nucleating” surfaces, screen then, and thereby completely prevent the ice formation.

This work is supported by the Russian Science Foundation (grant No. 21-14-00268).

Biography

Alexei V. Finkelstein:

- Graduated with honors from the Moscow Phys.-Tech. (1970). Ph.D. (1976); D.Sc. (1991).
- Since 1970, member of the Laboratory of Protein Physics (then headed by Prof. O.B. Ptitsyn) at the Institute of Protein Research, Russian Academy of Sciences. Heads this Laboratory since 1999.
- Professor at the Moscow Lomonosov University since 1998. Soros Professor (2001).
- Author of ~300 papers, of a book "Protein Physics", published in Russian (7 editions), English (2 editions), Chinese (2 editions), and of a book "Physics of Protein Molecules" (in Russian).
- Citation index: 11000, Hirsch index: 50.
- Expertise: Protein physics; theory of protein structures, folding and design; structural transitions in proteins and amyloids; antifreeze proteins and ice nucleators, phase transitions; force fields; molecular biology; bioinformatics.
- Awards from FIRCA, INTAS, CASP, HHMI (3 times), NWO, etc. State Prize of Russia in Science & Technology (1999).
- Elected to the Russian Academy of Sciences (2008).

Activation of inactive enzymes through biochemical and evolutionary approaches

Eri Tabata

Department of Chemistry and Life Science, Kogakuin University, Japan

Chitin, a polymer of *N*-acetyl-D-glucosamine (GlcNAc), functions as a major structural component in crustaceans, insects, and fungi and is the second most abundant polysaccharide in nature. While chitin production is absent in mammals, humans and mice express two active chitinases, chitotriosidase (Chit1) and acidic chitinase (Chia). Chia, characterized by its acidic isoelectric point, has garnered attention due to its altered expression in various human pathological conditions, including asthma and allergic inflammation. In certain animals, such as cattle (herbivores), low levels of Chia expression and chitinolytic activity have been observed, suggesting a potential link between feeding behavior and enzyme activity. We identified a specific amino acid substitution (H128R) that led to the inactivation of Chia in cattle. By creating mouse-cattle chimeric and mutant Chia proteins, we found that introducing the H128R substitution activated the cattle Chia enzyme. Notably, histidine at position 128 is conserved in many bovid species. It is associated with low chitinase activity, while a few bovid species that consume insects retain arginine at this position, resulting in Chia proteins with high enzymatic activity. Our findings highlight the significance of a single amino acid substitution in activating cattle Chia and shed light on the molecular evolution of Chia in herbivorous species. Chia-deficient mice accumulate chitin in the lungs and develop age-dependent fibrosis, but the transgenic expression of Chia relieves this condition in deficient mice. Therefore, this study allows the creation of highly active Chia that can be used to treat lung diseases.

Biography

Eri Tabata completed her Ph.D. at Kogakuin University in 2020. She is the Japan Society for the Promotion of Science (PD) research fellow. She has published eight peer-reviewed papers as the first author in high-quality journals, including Molecular Biology and Evolution (IF: 10.7), iScience (IF: 6.107) and Scientific Reports (IF: 4.6) with 226 citations (ref. Scopus).

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In-situ and transported nickel-rich regolith in the Bavanat region, SW of Iran: Constraints from geochemistry and mineralogy

Soqra Rasti and **Mohamad Ali Rajabzadeh**

Shiraz University, Iran

A nickel-rich regolith outcrops discontinuously between the Sedimentary Zagros Orogenic (SZO) and Metamorphic Sanandaj-Sirjan (MSS) belts in Fars province, southwest Iran. These mineral deposits are the only known Ni-bearing soils in Iran that can be divided into two groups including *in-situ* soils and transported soils. An undisturbed Nickel-bearing soil profile from bottom to top, reveals the following sequence: protolith, hard and soft saprolite, and oxide horizons. In some places, part of the profile of transported regolith, especially the oxide horizon has moved downslope due to landslide, slip, creep, and likely faulting. The parent rock is a highly serpentinized harzburgite containing relicts of olivine and orthopyroxene. In the transition from the hard saprolite to the oxide horizon, the proportions of hematite, goethite, talc, dolomite, and quartz increase, while chlorite, olivine, serpentine, and pyroxene decrease. Nickel concentration gradually increases upwards the laterite profiles, reaching 1.2 wt% in the oxide horizon. SEM-EDS data provide evidence that nickel released from serpentine group minerals in the parent rock, has been concentrated in the new formed minerals mainly hematite of the oxide horizon. The isotopic fractionation of nickel along the soil profiles is controlled by the circulation of meteoric water, the intensity of weathering, and the presence of secondary minerals. Based on chondrite-normalized REE patterns, the limonitic sample shows flat chondrite-normalized Rare Earth elements (REEs) patterns, while the other samples characterize light REE-enriched patterns; the same as the parent rock suggesting that the REE fractionation process in the limonitic sample is independent of the REE in the parent rock. The highest REEs are concentrated because of the presence of clay minerals and Fe-Mn oxides. This research offers valuable insights into the genesis and geochemical characteristics of the nickel-rich regolith in the Bavanat region. The findings highlight the potential of this unique deposit for future exploration and exploitation of nickel resources.

Biography

Soqra Rasti has completed her B.Sc. in geology, master's and Ph.D. degrees in economic geology at Shiraz University, Iran. Her master's dissertation focused on the mineralization of Iron deposits in the Dehbid metasedimentary rocks, Fars Province, Iran. Her Ph.D. thesis included detailed geological, mineralogical, geochemical, and biogeochemical studies of the Ni laterite deposits in NE of Fars Province, Iran. Furthermore, she completed fellowship research with Dr. Cecile Quantin at Université Paris Saclay, France (2018) in the GEOPS Laboratory. Her fellowship concentrated on mineralogy, geochemistry, and Ni isotopes of Ni-rich regolith in the Bavanat region. This fellowship provided her a unique opportunity to be involved in high-level research activities at GEOPS Laboratory and learn practical knowledge about AAS, ICP, XRD, XRF, SEM-EDS, and MC-ICP-MS techniques. She has a diverse knowledge base beyond the focus of her Ph.D. program. Through various research projects and practical work in the field., she learned 2D and 3D modeling of mineral deposits using various software packages including Datamine and Surpac parallels to GCDkit, X'Pert, MinPet, ENVI, ArcGIS, CanvasX, Latex, Matlab, Google Earth Engine, Geolog, and CorelDraw. She has participated in numerous conference presentations around the world (Norway, Austria, Germany, France). As a young researcher, she has published 24 papers in journals and conference proceedings for the last few years. She enjoys all aspects of research and she very much interested in carrying out her research in such a cutting-edge field.

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Utilizing choline chloride-containing DESs to extract value-added compounds from tomato pomace and incorporating them into cosmetic emulsion formulations

Liudmyla Khrokalo and **Victoria Vorobyova**

National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Ukraine

The aim was to evaluate the efficiency of environmentally-friendly choline chloride-based deep eutectic solvents (DESs) in extracting phenolic compounds and utilizing them in cosmetic products. The extraction process was optimized by sonication using. Two types of DESs were investigated, the first one was choline chloride: 1,2-propanediol (1:2 v/w) : water (10% w/w); the second was choline chloride : lactic acid (1:2 v/w) : water (10% w/w). The choline chloride is chosen as hydrogen bond acceptor due to its low cost, low toxicity, biodegradability, and biocompatibility, meanwhile, D,L-lactic acid and 1,2-propanediol are selected as hydrogen bond donors. Compounds are renewable and keep a liquid state at room temperature. To gauge the overall antioxidant capacity of the extracts, the phosphomolybdenum method was employed, while cyclic voltammetry was utilized to evaluate the redox potential. Additionally, the ζ-potential, colloidal stability, and antioxidant activity of the final cosmetic product were examined. The tomato pomace extracts were found to contain substantial quantities (26–37% from total amount) of phenolic acids and flavanols. Chlorogenic acid emerged as the predominant phenolic compound within the tomato pomace extracts, ranging 37.23–52.33 µg/g. The total antioxidant activity of extracts displayed variation from 408 to 511.18 µg/g. Choline chloride-based DESs exhibited notably low oxidation potential values. ζ-potential ranged from –0.0102 to –0.0594 mV, that is showed the middle stability of emulsions in cosmetic product. Upon assessment, it was determined that the antioxidant hierarchy within the cosmetic emulsions was as follows: emulsions containing extracts obtained from choline chloride: lactic acid deep eutectic solvent demonstrated the highest efficacy, followed by emulsions incorporating extracts from choline chloride:1,2-propanediol deep eutectic solvent. Moreover, the antibacterial and antifungal activities of these cosmetic emulsions were evaluated against *Bacillus subtilis* (poorly expressed), *Escherichia coli* (not registered) and *Candida albicans* (excellent expressed).

Biography

Dr. Liudmyla Khrokalo currently holds the position of Associate Professor in the Department of Physical Chemistry at the National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" (KPI). She was born in 1976 in Sumy Region. After receiving an Honors Diploma of Sumy Pedagogical Institute, she enrolled in a PhD at Kyiv National Taras Shevchenko University (KNU), focusing her research on Biology and Ecology. In 2005-2008, she worked as a lecturer at National Agricultural University of Ukraine. Since 2008, Liudmyla has been employed at KPI and provided research and teaching in Biochemistry, Enzymology, Nanochemistry, and Green Chemistry. In 2012–2014, she participated in Bilateral Ukrainian-Indian research projects, received academic mobility grants from Erasmus in 2006, 2016, and 2023, DAAD grant focusing on biocatalysis and one-pot flow technology. She has at total 130 publications.

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