The South African Chemical Institute

Promoting chemistry, chemists, the chemical industry and chemical education in South Africa

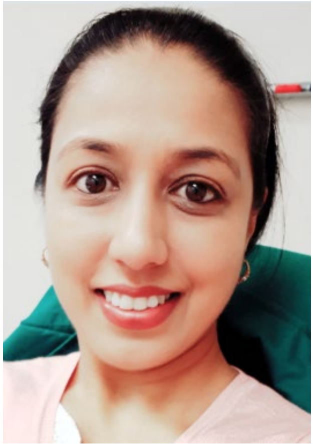
INORGANIC AND CARMAN 2024

2 - 6 June 2024
Champagne Sports Resort

Programme and Abstracts

Contents

Welcome!



On behalf of the local organising committee, I welcome you to Champagne Sports Resort for the 2024 SACI Inorganic and Carman Conference that will be held over the next four days from 2-6 June 2024. It has been six years since the last conference which was held in 2017 in Cape Town. The pandemic robbed us of two meetings! Hence, we will endeavour to make a refreshed start at ruKhahlamba-Drakensberg Park which is one of two UNESCO World Heritage Sites in South Africa.

Thank you to all the delegates for participating – without your contribution and attendance, there would be no meeting. The SACI 2024 Inorganic and Carman Conference is a momentous event on the South African Chemical Institute's (SACI) calendar. This is a platform for local as well as international researchers, including emerging and young career chemists, technologists and entrepreneurs to showcase their research, and familiarise themselves with the latest advances and trends in the disciplines of both inorganic and physical chemistry. This year we have included related chemistries such as sustainable chemistry, green chemistry, computational chemistry, nanoscience and nanotechnology.

The scientific committee has curated a programme that has 3 plenary, 11 keynote and 4 invited talks by distinguished scholars in their respective research discipline. The programme also includes orals, flash poster presentations, and posters which encompass the conference theme, "Sustainability Challenges, Collaborative Solutions".

I want to thank and acknowledge all the sponsors and donors for their valuable financial support. Please do visit the stands and meet the representatives.

Use this time to discuss science, network, and make new contacts. I hope you will enjoy the conference and find it fruitful.

Best wishes,

Thishana Singh

(On behalf of the 2024 ICC LOC)

Committees

Local Organizing Committee

Dr Thishana Singh (Chair)
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Prof Bice Martincigh (Treasurer)
Prof Vincent Nyamori (Technical Advisor)
Prof Neerish Revaprasadu (Chair: Scientific Panel)
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Prof Vincent Bisetty
Dr Thabang Mokhothu
Dr Pinkie Ntola
Dr Phindile Khoza
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Dr Nkululeko Damoyi
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Scientific Programme Committee

Prof Neerish Revaprasadu (Chair)
Prof Werner van Zyl
Prof Vincent Bisetty

Conference Secretariat and Webmaster

Mrs Laila Smith

Plenary Speakers

We are pleased to announce the following Plenary Speakers and the topics of their lectures.

Professor Nick Long
Imperial College
United Kingdom

Topic:
Organometallic-enhanced nanoelectronics and solar cells

Nick Long holds the Sir Edward Frankland BP Endowed Chair in Inorganic Chemistry at Imperial College London. He is a leader in applied synthetic inorganic and organometallic chemistry, with research interests focussing on transition metal and lanthanide chemistry for the synthesis of functional electronic and renewable energy materials, homogeneous catalysts and probes for biomedical imaging. He has over 300 publications, with around 14000 citations, an h-index of 56, and i10-index of 160. His work has recently been recognised by a Royal Society Wolfson Merit Award (2018), the Royal Society of Chemistry Frankland Award (2020), and the Royal Society of Chemistry Interdisciplinary Prize (2023).

Professor Emmanuel Iwuoha
University of Western-Cape
South Afica

Topic:
Patterns in the engineering of smart functional materials for clean energy conversion

Prof Emmanuel Iwuoha is an NRF A-Rated Scientist and a SARChI Chair for NanoElectrochemistry and Sensor Technology, in the Department of Chemistry, University of the Western Cape (UWC). He was admitted as a Chartered Chemist (CChem) in 1990, a Fellow of the Royal Society of Chemistry (FRSC) in 1999, a Fellow of the African Academy of Sciences (FAAS) in 2018 and a Fellow of the Royal Society of South Africa (FRSSAf) in 2023. His research work focuses on the creation of novel smart functional nanomaterials for next-generation electroanalytical sensor, battery, supercapacitor and solar cell applications. His work has impact on the attainment of the UN SDG 3 on health and well-being for all and the UN SDG 7 on the accessibility and sustainability of energy. He has published over 365 research articles, given more than 72 plenary and keynote presentations and graduated 80 PhDs. Prof Iwuoha received the 2015 UWC Vice-Chancellor's Distinguished Researcher Award. In 2020, he was awarded the Honorary Fellow of the Royal Society of Chemistry (HonFRSC) Award – being one of the first two recipients in Africa; and the NRF Champion of Research Capacity Development and Transformation Award. He is a member of the advisory boards of the Journal of the American Chemical Society Gold (JACS Au), Analytical Chemistry and Bioelectrochemistry; an Associate Editor of NPJ Clean Water; and a Guest Editor for Nanomaterials, Materials Today Communication and Frontiers in Sensors.

Professor Sarah Haigh
University of Manchester
United Kingdom

Topic:
Dynamic behaviour of single atomic species and nanoparticle catalysts revealed by in-situ transmission electron microscopy

Sarah Haigh is a Professor of Materials Characterisation at the University of Manchester, UK. She is also Director of the bp International Centre for Advanced Materials, a $100M academic-industrial collaboration, and of the University of Manchester's electron microscopy centre which includes 31 electron microscopes. Her research interests centre on improving understanding of nanomaterials structure and properties using transmission electron microscope (TEM) imaging and analysis techniques. She is particularly interested in 2D materials and in developing in situ TEM imaging methods. She completed undergraduate and doctorate degrees in Material Science at the University of Oxford (2004 and 2008). She is an elected member of Livery of the Worshipful Company of Armourers and Brasiers. She has won several awards including Blavatnik Physical Sciences Medal (2021), Royal Society of Chemistry Analytical Sciences Award (2022), Institute of Materials Mineral and Mining Silver Medal and Rosenhain Medals (2013 and 2017). She has published over 200 peer reviewed journal papers as an independent academic, including 45 as corresponding author, and 5 book chapters (H-index = 62, over 17000 citations).

Keynote Speakers

Professor Catharine Esterhuysen
Stellenbosch University
South Africa

Topic:
The role of noncovalent interactions in the properties of porous compounds

After completing a PhD in crystallography under the supervision of Gert Kruger at the Rand Afrikaans University in Johannesburg, South Africa, Catharine Esterhuysen joined Stellenbosch University in 2000. During her studies she developed an interest in computational chemistry, which she was able to develop through Alexander von Humboldt fellowships with Gernot Frenking in Marburg and Tim Clark at Erlangen. Her main research focus is the study of intermolecular interactions, combining her knowledge of computational chemistry and crystallography to explain unusual interactions and their role in the properties of materials. She has served on numerous committees and editorial boards, including as president of the South African Crystallographic Society and Associate Editor at New Journal of Chemistry.

Professor Gregory Smith
University of Cape Town
South Africa

Topic:
Visible light-induced bioorganometallic chemistry: Illuminating new frontiers

Greg Smith is a Professor of Inorganic Chemistry at the University of Cape Town. He obtained his undergraduate degree at the University of Natal, Pietermaritzburg, South Africa (SA) and went on to complete his MSc and PhD on the synthesis of metal-containing polymers and dendrimers as olefin transformation catalysts, under the supervision of Prof. Selwyn Mapolie at the University of the Western Cape (SA). He later joined the University of Bristol (UK) as a Postdoctoral Fellow with Prof. Ian Manners. His research interests in the discipline of Organometallic Chemistry, a subset of Inorganic Chemistry, investigates the synthesis of small molecule and macromolecular organometallic complexes. His primary activities are the development of Platinum Group Metal (PGM)-based complexes, with two broad themes/applications, aimed at the beneficiation of PGM resources available in South Africa. The first theme centres on the use of the organometallic compounds as homogeneous catalysts, whilst the second theme entails investigations into the application of organometallic complexes as chemotherapeutic agents.

Professor Lydia Rhyman
University of Mauritius
Mauritius

Topic:
Molecular insights into inorganic complexes using computational chemistry

Lydia Rhyman is a researcher in the Computational Chemistry Group of the University of Mauritius, Mauritius and the University of Johannesburg, South Africa. She was awarded a PhD in Computational Chemistry in 2013. She is an Affiliate of the African Academy of Sciences, a member of the Royal Society of Chemistry and a Global Young Academy member. She is also a committee member of the Commonwealth Chemistry Early Career Network representing the Africa region. Her research interest lies in the use of Computational Chemistry to solve chemistry and interdisciplinary problems. She is involved in promoting Computational Chemistry in Africa and science education and she also raises awareness on responsible research practices and integrity. She is active in the organisation of conferences, seminars, workshops and outreach activities. To date she has 135 publications, 4 book chapters and 1 patent.

Professor Kristian Brandt
University of Copenhagen
Denmark

Topic:
Metal-driven co-selection of antibiotic resistance

Kristian Koefoed Brandt leads the Environmental Microbiology Research Group at Department of Plant and Environmental Sciences, University of Copenhagen (Denmark). He holds a PhD degree in microbial ecology (1998) from Aarhus University, Denmark. He has worked as a postdoctoral fellow at the Royal Veterinary and Agricultural University (Denmark) and at the NSF Center for Microbial Ecology at Michigan State University (USA) and since then as an associate professor at Royal Veterinary and Agricultural University (2003-2006), University of Copenhagen (since 2007), and Sino-Danish Center (SDC) in Beijing, China (since 2013). Current research areas include the environmental dimension of antibiotic resistance, microbe-pollutant interactions, plant-soil-microbe interactions, bacterial community assembly processes, and bioavailability processes in environmental settings.

Professor Reinout Meijboom
University of Johannesburg
South Africa

Topic:
Digital manufacturing meets catalysis: some examples of 3D printing in chemistry

Reinout Meijboom was born and raised in the Netherlands. He studied chemistry at the University of Groningen where he completed his MSc research under Prof Jan Teuben. Subsequently, he moved to Cape Town to pursue his PhD in organometallic chemistry under the supervision of Prof John R. Moss. Following his PhD, he pursued a post-doctoral fellowship with Prof Andre Roodt at the then Rand Afrikaans University (currently University of Johannesburg) and the University of the Free State. Reinout took up the position of Senior Lecturer at the University of Johannesburg in 2008. He changed his research direction towards heterogeneous catalysis while pursuing the crystallography of silver coordination compounds. He raised through the ranks at UJ to full professor and was the former head of department. Since October 2021, he serves as the Vice-Dean for Research in the Faculty of Science. His current research interests are high throughput experimentation, heterogeneous catalysis, and building Open Source hardware for Chemistry. The latter includes the design and construction of robotic systems for synthetic chemistry. Reinout has published over 200 research papers.

Professor Tiina Leiviskä
University of Oulu
Finland

Topic:
Combined methods of preconcentration and degradation for removal of per- and polyfluoroalkyl substances

Tiina Leiviskä is a Professor in the Chemical Process Engineering unit at University of Oulu, Finland. Tiina Leiviskä obtained her D. Sc. (Tech.) degree in Water Resources Engineering in 2010 and a M.Sc. degree in Chemistry in 2001, both from the University of Oulu. Currently, she is leading the industrial water research group. Her research interests include bio-based water treatment materials, coagulation-flocculation, ion exchange, adsorption, degradation of refractory organics and recovery of valuable components.

Professor Nosipho Moloto
University of the Witwatersrand
South Africa

Topic:
Nanocrystals: Breaking boundaries in alkaline water splitting

Nosipho Moloto is a full Professor of Inorganic Chemistry at the University of the Witwatersrand (WITS) where she holds the NEDBANK-DSI SARChI Chair in Energy Materials. Nosipho obtained her Masters in Nanotechnology studying quantum dots at the University of Zululand with links to the University of Manchester. She then obtained a PhD in Nanotechnology still working on quantum dots from the CSIR/WITS (2008-2010. This was followed by a postdoctoral stint at the Massachusetts Institute of Technology in the US (2010). She was a visiting senior scientist at the Institute for Photonic Sciences (Spain) working with the Functional Optoelectronic Nanomaterials Group. In 2014 Nosipho was awarded the Distinguished Young Woman in Science (Physical and Engineering Sciences) by the Ministry of Science and Technology (South Africa) and 2016 she was awarded the NRF Research Excellence Award for Early Career/Emerging Researchers and recently, 2023, the NSTF-South32 Award for Engineering Research Capacity Development. From WITS University, she has received the Friedel Sellschop Research Excellence Award for emerging researchers and the Faculty of Science Supervision Award in 2021. Nosipho is an associate editor for the South African Journal of Chemistry (Nanotechnology) and she has been on selection committees for the Lindau Laureates Meetings (Germany), Serrapiheira Institute’s The Science Program (Brazil) and the King Faisal Prize (UAE). Nosipho Moloto has co-authored more than 100 papers on the syntheses of semiconductor nanomaterials for water, energy, biomedical and sensor applications.

Professor Stephen Ojwach
University of KwaZulu-Natal
South Africa

Topic:
Probing the cytotoxicity of Pd(II) and Ru(II) metal complexes through the lenses of substitution kinetics and biomolecular interactions

Stephen Ojwach obtained his BScHons degree in Chemistry from the University of Nairobi, MSc and PhD degrees in Inorganic Chemistry (with a bias in organometallic chemistry and homogeneous catalysis) from the University of Western Cape and University Johannesburg (South Africa) respectively. Prof Ojwach is currently a Professor of Inorganic Chemistry at the University of KwaZulu-Natal (South Africa). His research area is mainly on the design of transition metal complexes, investigation of their coordination behavior and applications as catalysts in various organic transformations and sustainable processes, bioinorganic chemistry. He has published over 120 research articles in the fields of Inorganic Chemistry, Organometallic Chemistry, Catalysis and Bioinorganic Chemistry. He is currently an Associate Editor, RSC Advances, Royal Society of Chemistry.

Professor Zenixole R. Tshentu
Nelson Mandela University
South Africa

Topic:
Cushioning the global transition to clean energy through sustainable sourcing and processing of fuel oils

Zenixole R. Tshentu Research Excellence Award from NMU (2015) and a Raikes Medal from South African Chemical Institute (2016). He has experience in solid state and solution studies of transition metal complexes as well as using inorganic/organic polymer materials in heterogeneous catalysis and in separation technology. He has been involved in several projects including designing catalysts and adsorbents for desulfurization and denitrogenation of fuels as well as designing selective reagents for separation of base metals and platinum group metals. His pursuit of knowledge is in principles that drive towards selectivity and specificity in chemical systems with the aim of applying them in greening of fuel products, sustainable processing of fuel oils and beneficiation of mineral resources as well as in valorisation of secondary products.

Dr Malik Dilshad Khan
National Research Foundation
South Africa

Topic:
Metal-organic precursor-derived functional nanomaterials for energy generation and storage applications

Dr. Malik Dilshad Khan is an NRF-rated researcher in the nanotechnology group at the University of Zululand. He obtained his Ph.D. from the University of Zululand in 2018 under the supervision of Prof. Neerish Revaprasadu. During his Ph.D., he visited the University of Manchester for a year and was trained in state-of-the-art instruments and synthetic techniques. He is an expert in designing and synthesizing suitable metal organic precursors for functional nanomaterials via different routes and thin films by AACVD. His research interests include synthesizing 2-dimensional materials, multinary metal oxides, sulfides, selenides, phosphides, intermetallic alloys and solid solutions for HER, OER, ORR and supercapacitance. He has also visited the Institute of Physical Chemistry in Poland and worked on the deposition of nanomaterials at the liquid-liquid interfaces and investigated their ORR via SECM. He has co-authored over 80 articles in well-reputed journals, 6 book chapters and a patent. He is also the editor of Nanosciences: Specialist Periodical Reports, a book series by RSC publishers.

Professor Roman Gorbachev
University of Manchester
United Kingdom

Topic:
Recent progress in nanotechnology van der Waals heterostructures

Roman Gorbachev's research area is experimental condensed matter physics, with an emphasis on fabrication of nanoscale low-dimensional devices. The recent availability of novel nanoscale materials, such as atomically thin 2-dimensional crystals and nanowires has enabled the assembly and study of composite electronics and mechanical devices, as well as the exploration of fundamental physics in these low-dimensional systems. The use of modern state-of-the-art semiconductor device fabrication techniques and the development of new methods of material synthesis/manipulation are essential parts of this research, which gives an ample space to explore the new physical phenomena and can bring an impact to future technologies. To date he has published over 85 peer-reviewed papers, attracting over 30,000 citations and h-index of 55 (Google Scholar).

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General Information

Conference Registration

Conference registration will take place on **Sunday 2nd June 2024** from 14h00 to 18h00. On Sunday registration will take place in the main foyer of Champagne Sports Resort.

Name Tags

Please wear your name tag at all times for access to the conference venue, meals and social functions.

Social Functions

All social functions mentioned below are included in the delegate registration fee.

2nd June 2024 – Welcome Reception in the pool area – 18h00 – 20h30. This is followed by a Market Menu dinner in the main dining room.

3rd June 2024 –Braai in the pool area at 18h30.

5th June 2024 – Gala Dinner, Sentinel – 18h30 - 22h00. Dress Code for the dinner is formal or traditional.

Please take note that two drinks tickets will be provided for each event and thereafter there will be a **cash bar** and only South African Rand will be accepted.

Presenters

All presenters must upload their presentations in Monks Cowl during the break (tea or lunch) prior to their presentation. The audio-visual technician will assist.

Posters

The Poster Sessions will be held on **Monday, 3rd June 2024** and **Tuesday, 4th June 2024** from 17h00 – 18h30. These sessions will be held in the Summit venue. Materials to place the posters on the poster boards will be provided. Posters can be put up after tea on Monday and must be removed at the conclusion of the poster session on Tuesday. Please do not remove or obscure the poster number. These are needed for judging purposes.

There will be judges scrutinizing the student posters during the poster session and the winner and runners-up will be announced on Thursday, 6th June 2024, at the closing ceremony.

Wireless/Internet/Fax/Photocopying

For those who require an internet station, faxing or photocopying, they can request assistance at the Reception area of Champagne Sports Resort. All charges for these facilities will be for the delegates own account. Wi-Fi is available throughout the hotel and conference venues.

Parking

Delegates arriving with their own vehicle can park at the grounds of resort.

Currency

Please note that only the South African Rand will be accepted. You can exchange any foreign currency at OR Tambo International Airport or at King Shaka International Airport. Should you wish to visit any bank during your stay, please note that the general banking hours in South Africa are 9h00 to 15h30 Mondays to Fridays, and 8h30 to 11h30 on Saturday mornings. Banks are closed on Sunday. Also note, the closest town to the Resort is Winterton, which is 25.9 km away and a 25-30 minute drive.

Weather

June in Southern Africa is late autumn or fall; hence, it is good to pack accordingly for the weather. The Central Drakenburg experiences mild weather conditions typically between 18-23 °C during the day and 9-15 °C at night, so we recommend bringing the appropriate clothing. If you have booked any of the activities offered by the Resort, please bring the appropriate attire.

Conference Contact Details

Should you require any other information or any assistance please do not hesitate to contact the conference secretariat on the numbers below.

Laila Smith
Conference Secretariat
SACI
Tel: +27 011 717 6705
Email: saci.chem@wits.ac.za
Website: https://www.saci.co.za/INORG2024/

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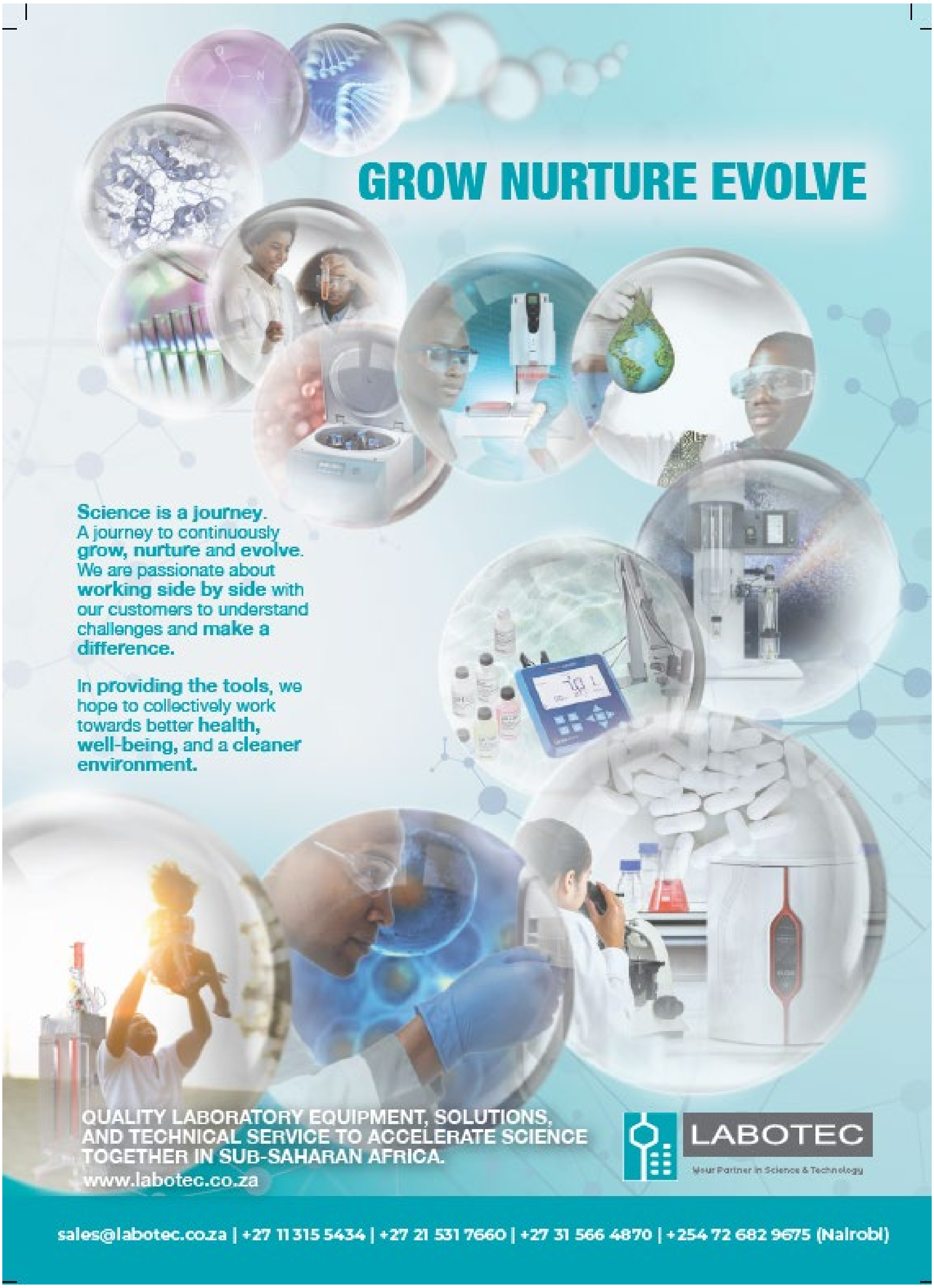

ACCREDITATION: ENSURING QUALITY AND SAFETY

The South African National Accreditation System (SANAS) is the national accreditation body responsible for carrying out internationally recognised and effective accreditations as mandated through the Accreditation for Conformity Assessment, Calibration and Good Laboratory Practice Act (Act 19 of 2006), in support of the public policy objectives including trade facilitation and economic growth.

It is recognised as a signatory to the International Laboratory Accreditation Cooperation (ILAC) Mutual Recognition Arrangements (MRAs), the International Accreditation Forum (IAF) Multilateral Arrangement (MLA), the African Accreditation Cooperation (AFRAC) MRA and the SADCA MRA for specific scopes. This recognition covers the following scopes and allows for SANAS accreditation to be accepted globally:

- Testing
- Calibration
- Medical Testing
- Management Systems Certification in the following sub-scopes:
  - Quality Management Systems (QMS)
  - Environmental Management Systems (EMS)
  -
  - Food Safety Management Systems (FSMS)
  - Occupational Health and Safety Management Systems (OH&SMS)
  - Energy Management Systems (EnMS)
- Product Certification
- Proficiency Testing
- Reference Materials Producers
- Medical Testing (ISO 15189)
- Inspection

SANAS has accredited just over two-thousand one-hundred and fifty-two Conformity assessment bodies (2,152) with three hundred and eight (308) Mechanical and Microbiological Testing Laboratories that plays an important role to increase access to goods and services of consistent and reliable quality and that meets safety standards.

These accredited Conformity Assessment Bodies build confidence that goods and services, processes, management systems and the work of individuals comply with national and international standards and regulations, also assist in the risk-management and decision making of manufacturers and regulators.

SANAS accreditation therefore contributes to the country's economic growth, as well as industry and government's objectives in terms the protection of health, safety, and the environment.

Read more about the services we offer visit our website: www.sanas.co.za

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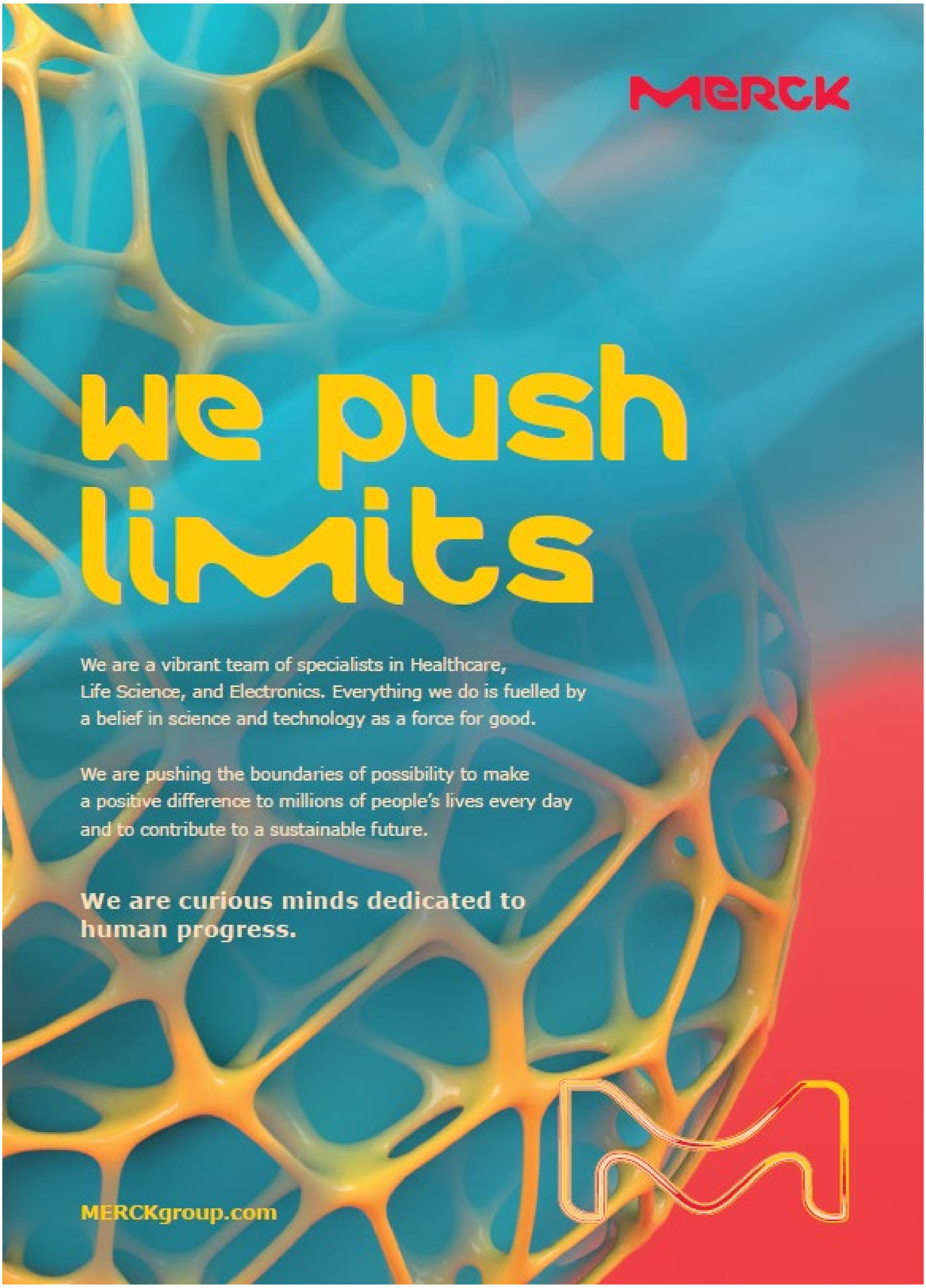

The Durban University of Technology (DUT) is a globally recognised University based in KwaZulu-Natal, comprising of seven campuses, with five in Durban and two in Pietermaritzburg, with a total of six faculties in Accounting & Informatics, Applied Sciences, Arts & Design, Engineering & the Built Environment, Health Sciences and Management Sciences.

According to the Times Higher Education World University Rankings, in 2023, DUT was ranked among the **top 600** universities globally.

DUT is also a member of the International Association of Universities, and DUT is at the forefront of higher education, technological training, research, and innovation. In alignment with DUT's strategy **ENVISION2030**, the University encourages its staff and students to become entrepreneurial and innovative.

At DUT, research and innovation are key to scientific and technological progress. More importantly, innovation is a catalyst in resolving society's deep and pressing socio-economic challenges while also supporting commercialisation. DUT has identified the following key research focus areas for research and innovation.

DUT RESEARCH FOCUS AREAS

- AFRICAN INDIGENOUS KNOWLEDGE SYSTEMS RESEARCH
- CENTRE FOR AFRICAN GOVERNANCE AND DEVELOPMENT (CAGD)
- COMPOSITE RESEARCH GROUP (CRG)
- COMPUTATIONAL MODELLING AND BIOANALYTICAL CHEMISTRY
- ENERGY
- ENZYME TECHNOLOGY
- FOOD & NUTRITION SECURITY
- GENDER JUSTICE AND HUMAN HEALTH DEVELOPMENT (GJHHD)
- GLOBAL HEALTH AND SUSTAINABILITY
- GREEN ENGINEERING
- ICT AND SOCIETY
- INSTITUTE FOR SYSTEM SCIENCE
- INTERNATIONAL CENTRE OF NONVIOLENCE (ICON)
- IWWT - INSTITUTE FOR WATER AND WASTEWATER TECHNOLOGY
- MANAGEMENT STUDIES
- MATERNAL HEALTH
- PLANT BIOTECHNOLOGY
- SPACE SCIENCE AND SMART GRID
- THE URBAN FUTURES CENTRE (UFC)
- TRANSFORMATION THROUGH THE ARTS AND DESIGN

FACULTY OF ACCOUNTING & INFORMATICS

FACULTY OF APPLIED SCIENCES

FACULTY OF ARTS & DESIGN

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FACULTY OF SCIENCE, AGRICULTURE AND ENGINEING
DEPARTMENT OF CHEMISTRY

The department of chemistry since its inception, the department has been engaged in imparting the highest level and quality of academic education. This department constitutes a 6-member faculty expertise in frontier level of research, the main areas of research being nanotechnology, homogeneous and heterogeneous catalysis, organometallics, polymer chemistry, analytical chemistry and environmental chemistry.

One of our key missions is to generate human resource of unmatchable quality. We provide under graduate and post-graduate programs with the aim of producing chemists with high professional competence, in carrying out research of both basic and applied nature. Currently, there are 8 M.Sc and 4 Ph.D. students.

Chemistry is the study of matter, its properties, how and why substances combine or separate to form other substances, and how substances interact with energy. Many people think of chemists as being white-coated scientists mixing strange liquids in a laboratory, but the truth is we are all chemists.with its rural and urban campuses.

Chemistry is part of everything in our lives. Every material in existence is made up of matter - even our own bodies. Chemistry is involved in everything we do, from growing and cooking food to cleaning our homes and bodies to launching a space shuttle. Chemistry is one of the physical sciences that help us to describe and explain our world.

DEGREE	MINIMUM REQUIREMENTS	DURATION
B.Sc.,	Matric: 30 Points Mathematics – 5, Physical Science – 4, English – 4	3
B.Sc., Honours	60% average mark from B.Sc., Chemistry 3rd level modules	1
M.Sc.,	B.Sc., Honours Chemistry degree	2
Ph.D.,	M.Sc., Chemistry degree	3

Switchboard: 035 902 6000 | **Reception:** 035 902 6646 | **Admissions:** 035 902 6178
Fax: 035 902 6027/33 | **Enquiries Email:** admissions@unizulu.ac.za | **Richards Bay Campus:** 035 902 6006

FACULTY CONTACT DETAILS:

Faculty of Science, Agriculture and Engineering - Department of Chemistry
Email: KhumaloMS@unizulu.ac.za | **Phone:** (035) 902 6649 | **Website:** https://www.science.unizulu.ac.za/chemistry/

Scientific Programme

Sunday, 2 June 2024

14.00-18.00	Registration and check-in
18.00-20.30	Welcome and dinner: Market Menu

Monday, 3 June 2024

7.00-8.30	Breakfast
8.45-9.00	**Opening & Welcome** – Thishana Singh
9.00-10.00	**Session 1 Chair: Neerish Revaprasadu** **Plenary 1: Nick Long** - Organometallic-enhanced nanoelectronics and solar cells (Imperial College, UK)
10.00-10.15	**Tribute to Prof Tony Ford** – Neil Coville and Bice Martincigh
10.15-10.40	TEA
10.45-11.15	**Session 2 Chair: Tshephiso Papo** **Keynote 1: Gregory Smith** - Visible light-induced bioorganometallic chemistry: Illuminating new frontiers (UCT)
11.15-11.35	**Oral 1: Kristy-Lyn Barry** - Synthesis, characterisation, DNA binding and cytotoxic studies of novel phenanthroline-derived oxovanadium(IV) complexes (UKZN)
11.35-11.55	**Oral 2: Nikoletta Bathori** - Solid-state crystalline structures of baclofen (CPUT)
11.55-12.25	**Invited 1: Nikolay Gerasimchuk** - Structural chemistry of cyanoximes (Missouri State Uni, USA)
12.25-12.55	**Keynote 2: Stephen Ojwach** - Probing the cytotoxicity of Pd(II) and Ru(II) metal complexes through the lenses of substitution kinetics and biomolecular interactions (UKZN)
13.00-13.55	LUNCH
14.00-14.30	**Session 3 Chair: Emmanuel Damoyi** **Keynote 3: Lydia Rhyman** – Molecular insights into inorganic complexes using computational chemistry (Uni Mauritius, Mauritius)
14.30-14.45	**Student 1: Ngonidzashe Ruwizhi** - Using computational drug design for the synthesis of NHC metallodrugs as potential anticancer and antimicrobial agents (UKZN)
14.45-15.00	**Student 2: Vitalis Mbayo** - Quantum chemical studies on antiviral drugs – an insight into antimicrobial resistance (UJ)
15.00-15.30	**Keynote 4: Kristian Brandt** – Metal-driven co-selection of antibiotic resistance (Uni Copenhagen, Denmark)
15.30-15.55	TEA
16.00-16.05	**Session 4 Chair: Mzamo Shozi**

16.05-16.10	**FP 1: Taryn Golding** - The multi-stage antiplasmodial activity and mechanistic investigation of ferrocenyl quinoline-benzimidazole molecular hybrids (UCT)
16.10-16.15	**FP 2: Mnqobi Zikode** - Development of N,O-donor earth abundant metal catalysts for the synthesis and depolymerization of poly(lactides) (UKZN)
16.15-16.20	**FP 3: Blessing Masora** - A computational study of mechanistic pathways for the design of a greener process in the production of quinoline-2-(1H)-one and its derivatives (UJ)
16.20-16.25	**FP 4: Ndivho Mphoshomali** - Synthesis, spectroscopic characterisation, and CO-release of Mn(I) tricarbonyl complexes, coordinated with biologically active amino-based ligands (TUT)
16.25-16.30	**FP 5: Mpho Ledwaba** - The integration of acid leaching with Metal-Organic Framework-based adsorption for the efficient extraction of platinum group metals (Mintek)
16.30-16.35	**FP 6: Korban Oosthuizen** - Metalate anion extraction for separation of cobalt(II) from nickel(II) and manganese(II) (SU)
16.35-16.40	**FP 7: Zizipho Ngayeka** - Synthesis and characterization of composite track-etched membranes for application in mine-waste waters (NMU)
16.40-16.45	**FP 8: Murendeni Ravele** - CuO nanoparticles functionalised graphitic carbon nitride for the degradation of ibuprofen in water (NWU)
16.45-16.50	**FP 9: Sarah Scott** - Synthesis and study of thiolato-gold(I) complexes as anticancer agents (SU)
17.00-18.30	POSTER VIEWING
18.30	Dinner: Braai

Tuesday, 4 June 2024

7.00-8.30	Breakfast
8.45-9.45	**Session 5 Chair: Vincent Bisetty** **Plenary 2: Emmanuel Iwuoha** - Patterns in the engineering of smart functional materials for clean energy conversion (UWC)
9.45-10.10	TEA
10.15-10.45	**Session 6 Chair: Lindelani Qwabe** **Invited 2: Sreekantha Jonnalagadda** - Novel nanocomposites and mixed oxide material as recyclable catalysts and other applications (UKZN)
10.45-11.05	**Oral 3: Vladimir Azov** - Pd-catalyzed cross-couplings in the synthesis of non-canonical amino acids for the use in hydrogelators (UFS)
11.05-11.20	**Oral 4: Adeniyi Ogunlaja** - Enhanced HDS and HYD activity of sulfide Co-ligand/Mo catalyst supported on γ-alumina (NMU)
11.20-11.40	**Oral 5: William Moloto** - Visible light active metal supported TiO_2/C nanohybrids for photocatalytic removal of organic compounds in water (Mintek)

11.40-12.00	**Oral 6: Eric Ayom** - Dithiophosphonates as versatile precursors to the formation of nickel sulphides and phosphides towards water splitting (UNIZULU)
12.00-12.30	**Keynote 5: Nosipho Moloto** - Nanocrystals: Breaking boundaries in alkaline water splitting (Wits)
12.30-13.25	LUNCH
13.30-14.00	**Session 7 Chair: Werner van Zyl** **Invited 3: Abdou Lachgar** - Photocatalytic green hydrogen production using semiconductor heterojunctions (Wake Forest Uni, USA)
14.00-14.20	**Oral 7: Manoko Maubane-Nkadimeng** - Waste to value: How can we effectively convert waste into useful materials? (Wits)
14.20-14.40	**Oral 8: Henrietta Langmi** - Synthesis and properties of metal-organic frameworks derived from waste feedstock (UP)
14.40-14.55	**Student 3: Caren Kurgat** - Photodegradation of tetracycline by a bismuth oxyiodide/red phosphorus photocatalyst (UKZN)
14.55-15.10	**Student 4: Brian Chabalala** - Green approach for the synthesis of ZnO-Ag using β-cyclodextrin and honey for photo-catalytic degradation of bromophenol blue (Mintek)
15.10-15.40	**Keynote 6: Tiina Leiviskä** - Combined methods of preconcentration and degradation for removal of per- and polyfluoroalkyl substances (PFAS) (Uni Oulu, Finland)
15.40-16.00	TEA
16.00-16.05	**Session 8 Chair: Pinky Ntola**
16.05-16.10	**FP 10: Leandre van der Merwe** - Targeting breast cancer with novel organometallic complexes (SU)
16.10-16.15	**FP 11: Ndumiso Nkosi** - Synthesis of zinc-based nanoparticles rested on multiwalled carbon nanotubes for antimicrobial and photocatalytic activity (UKZN)
16.15-16.20	**FP 12: Azeezat Rasheed-Adeleke** - Synthesis and photocatalytic performance of $Ag_3PO_3/ZnFe_2O_4$ composite on tetracycline in water (NWU)
16.20-16.25	**FP 13: Karabo Khoza** - The effect of different stabilisers on stability and photothermal profiling of gold nanorods (UJ)
16.25-16.30	**FP 14: Keaoleboga Mosupi** - Supercritical carbon dioxide synthesis of iron-based metal organic frameworks (UP)
16.30-16.35	**FP 15: Malcolm Ndlovu** - Synthesis and study of novel organometallic carbazole derivatives as heat shock protein inhibitors for malaria (SU)
16.35-16.40	**FP 16: Sandisiwe Mdoda** - Synthesis, characterisation and anticancer activity of pyrazole-based ruthenium(II) arene complexes (UCT)
16.40-16.45	**FP 17: Thabang Lebepe** - Synthesis of graphene oxide-gold nanorods nanocomposite-porphyrin conjugate for improved dual cancer phototherapy performance (UJ)
16.45-16.50	**FP 18: Adela Madaree** – Functionalised graphitic carbon nitride nanohybrids for the piezoelectric-photocatalytic degradation of organic contaminants in wastewater (UKZN)

17.00-18.30	POSTER VIEWING
18.30	Dinner: Buffet

Wednesday, 5 June 2024

7.00-8.30	Breakfast
8.45-9.15 9.15 – 9.45	**Session 9 Chair: Zenixole Tshentu** **Keynote 7: Catharine Esterhuysen** - The role of noncovalent interactions in the properties of porous compounds (SU) **Keynote 8: Roman Gorbachev** - Recent progress in nanotechnology van der Waals heterostructures (Uni Manchester, UK)
9.45-10.10	TEA
10.15-10.45	**Session 10 Chair: Cheslin Moodley** **Keynote 9: Zenixole Tshentu** - Cushioning the global transition to clean energy through sustainable sourcing and processing of fuel oils (NMU)
10.45-11.00	**Student 5: Mahdiyeh Mohammadzadeh** - Adsorption of pharma-ceuticals from municipal wastewater effluent by cost-effective magnetite-pine bark biosorbent in a pilot-scale column (Uni Oulu)
11.00-11.15	**Student 6: Fulufhelo Tshikhudo** - Synthesis of substituted triazines and their investigation as corrosion inhibitors on aluminum in 1M HCl: Experimental and computational approach (UniVen)
11.15-11.30	**Student 7: Lesetja Ramoba** - Schiff-base pyrazole chelator ligands coordinated to the fac-$[Re(CO)_3]^+$ synthon: synthesis, crystallography and in vitro studies (TUT)
11.30-11.45	**Student 8: Opeyemi Iresemowo** - Selective electrochemical detection of ciprofloxacin with functionalised reduced graphene oxide/strontium oxide-palladium nanocomposites (UKZN)
11.45-12.05	**Oral 9: Olatunde Olalekana** - Construction of S-Scheme 0D/3D $Cd_{0.5}Zn_{0.5}S/CeO_2$ heterojunction for the degradation of Cr(VI) and antibiotics (NWU)
12.10-13.30	LUNCH
13.30-18.30	Activities, Games, Free Time
18.30-22.00	GALA DINNER

Thursday, 6 June 2024

07.00-08.45	Breakfast
09.00-10.00	**Session 11 Chair: Prof Vincent Nyamori** **Plenary 3: Sarah Haigh** - Dynamic behaviour of single atomic species and nanoparticle catalysts revealed by in-situ transmission electron microscopy (Uni Manchester, UK)
10.00-10.25	TEA
10.30-11.00	**Session 12 Chair: Phindile Khoza**

	Keynote 10: Malik Khan - Metal-organic precursor-derived functional nanomaterials for energy generation and storage applications (UNIZULU)
11.00-11.20	**Oral 10: Christophe Ndamyabera** - Thermochromic aluminium-based fumarate MOF and its kinetic adsorption for nitrogen containing compounds (UP)
11.20-11.40	**Oral 11: Nolwazi Nombona** - Cellulose composite films as flexible electronics and adsorbent materials (UP)
11.40-12.10	**Invited 4: Matthew Davies** - Understanding the photochemistry of perovskites for photovoltaics (Swansea Uni, UK)
12.10-12.40	**Keynote 11: Reinout Meijboom** - Digital manufacturing meets catalysis: some examples of 3D printing in chemistry (UJ)
12.40-13.00	Closing remarks
13.00-14.00	LUNCH & DEPARTURE

Poster Presentations

Abstract Number	**Presenter**	**Poster Title**
P1	William Chu	Development of novel ruthenium-based metallodrugs for application in photodynamic therapy
P2	Sarah Scott	Synthesis and study of thiolato-gold(I) complexes as anticancer agents
P3	Monika Nowakowska	Spectroscopic and computational pH study of Ni(II) and Pd(II) Pyrrole-imine chelates with human serum albumin
P4	Mabu Matlou	Anticancer activities of Re(I) tricarbonyl complexes with N,O-bidentate ligands: synthesis, in vitro and in silico biological evaluation
P5	Nqobile Ndlangamandla	Synthesis, characterization, DFT, molecular docking and antimalarial studies of novel salen-based ruthenium complexes
P6	Taryn Golding	The multi-stage antiplasmodial activity and mechanistic investigation of ferrocenyl quinoline-benzimidazole molecular hybrids
P7	Makhosonke Ngcobo	Fine-tuning the chemical and physical properties of zeolitic catalysts for the ethanol dehydration process to form ethylene
P8	Mnqobi Zikode	Development of N,O-donor earth abundant metal catalysts for the synthesis and depolymerization of poly(lactides)
P9	Boitumelo Nthapo	Re^{I} tricarbonyl modalities with newly designed and synthesized *N,N'*-pyrazole ligand frameworks as potential anticancer drugs
P10	Mangaliso Goge	Synthesis, characterization, and biological studies of Pt(II) complexes with bidentate iminopyridine ligands
P11	Ndivho Mphoshomali	Synthesis, spectroscopic characterisation, and CO-release of Mn(I) tricarbonyl complexes, coordinated with biologically active amino-based ligands
P12	Petrus Prinsloo	Completing the picture – The halogenated benzoylanilides
P13	Chakanaka Mungwari	Optimization of maceration technique for extraction and characterization of Mimosa Wattle (*Acacia Mearnsii*) tree bark constituents
P14	Fidelis Chigondo	Green synthesis of silver nanoparticles and the evaluation of their antimicrobial activity
P15	Blessing Masora	A computational study of mechanistic pathways for the design of a greener process in the production of quinolin-2-(1H)-one and its derivatives

P16	Nonkosi Matinise	Development and use of novel ligands for selective separation of Co^{2+}, Ni^{2+}, and Mn^{2+} by solvent extraction via inner sphere coordination
P17	Solomon Oloyede	Synthesis of metal-organic framework and ternary quantum dot composites as electrochemical sensor for the detection of bisphenol A
P18	Nthabeleng Hlapisi	Biogenic synthesis of silver nanoparticles and their interaction studies with bovine serum albumin
P19	Segun Oladipo	Copper(II) complexes derived from naphthalene-based halogenated Schiff bases: Synthesis, structural analysis, DFT studies and biological activities
P20	Allen Tauya Gordon	Copper(II)-photocatalyzed hydrocarboxylation of Schiff bases with CO_2
P21	Korban Oosthuizen	Metalate anion extraction for separation of cobalt(II) from nickel(II) and manganese(II)
P22	Munyaradzi Shumba	Utilization of reduced graphene oxide intercalated Mn/Co bimetallic system for poly matrix pollutant electrodetection
P23	Thabang Lebepe	Synthesis of graphene oxide-gold nanorods nanocomposite-porphyrin conjugate for improved dual cancer phototherapy performance
P24	Karabo Khoza	The effect of different stabilisers on stability and photothermal profiling of gold nanorods
P25	Kgaugelo Tapala	Crystal structure, Hirshfeld surface analysis and antiproliferative activities of ruthenium and osmium complexes with tropolonate ligands
P26	Mpho Ledwaba	The integration of acid leaching with metal-organic framework-based adsorption for the efficient extraction of platinum group metals
P27	Adela Madaree	Functionalised graphitic carbon nitride nanohybrids for the piezoelectric-photocatalytic degradation of organic contaminants in wastewater
P28	Nirvashi Autar	Towards anticancer studies: Redox-mediated interactions of dansyl-based diruthenium complexes with biological molecules, GSH and ROS
P29	Nabeelah Sarang	Synthesis and characterisation of meso-substituted pyrrole-based metal complexes as potential DNA binders
P30	Ndumiso Nkosi	Synthesis and characterization of water-soluble nanoparticles and their application in fluorescence imaging
P31	Vuyiseka Qomfo	The synthesis, X-ray characterization, spectroscopic and Hirschfield surface analysis of dimeric metal centers featuring phenacyl-esters

P32	Sibusiso Sithole	Antimicrobial activity of rhenium(I) tricarbonyl 2-(pyridin-2-yl) quinoline complexes coordinated with various azoles
P33	Sandile Khoza	Solventless synthesis of cation-doped 2D-$CoSe_2$ nanomaterials for water splitting and supercapacitance
P34	Sandisiwe Mdoda	Synthesis, characterisation and anticancer activity of pyrazole-based ruthenium(II) arene complexes
P35	Ferdinand Misakabu	Novel *ansa*-bis(indenyl) ligands for transition metal complexes: synthesis and characterisation
P36	Tshepang Mohale	Application of deep eutectic solvents as extraction media for azeotropes
P37	Keotshepile Malebadi	Synthesis, structural, morphological and optical characterization of gC_3N_4/ZnO as a potential photocatalyst
P38	Murendeni Ravele	CuO nanoparticles functionalised graphitic carbon nitride for the degradation of ibuprofen in water
P39	Mathato Motaung	DFT calculations of Ag doped MoS_2 nanocomposite biosensor for highly sensitive detection of pathogens
P40	Keaoleboga Mosupi	Supercritical carbon dioxide synthesis of iron-based metal organic frameworks
P41	Nwabisa Khethula	Optimum route for the preparation of activated zeolitic imidazolate framework-derived carbons for CO_2 adsorption
P42	Lijo Mona	Structural, morphological and spectroscopic properties of magnetite quantum dots: Effects of temperature and time
P43	Mhlengi Msomi	A physicochemical investigation of the mechanism of formation of Cu_2S in insulation materials in liquid-filled transformers
P44	Deogratius Maiga	Development, optimization and performance of a novel reactor for acid mine drainage remediation using batches of natural substrates
P45	Siphosethu Maqinana	Synthesis of Fe_3O_4 and silica-supported N^O chelating agents towards the removal of Cd(II), Cr(VI), and Pb(II) cations from aqueous solutions
P46	Azeezat Rasheed-Adeleke	Synthesis and photocatalytic performance of $Ag_3PO_3/ZnFe_2O_4$ composite on tetracycline in water
P47	Henrietta Langmi	Water electrolysis for green hydrogen production using metal organic frameworks
P48	Siziwe Gqoba	1D/3D PANI/WS2 composite for highly selective room temperature sensing of ammonia vapours

P49	Malcolm Ndlovu	Synthesis and study of novel organometallic carbazole derivatives as heat shock protein inhibitors for malaria
P50	Leandre van der Merwe	Targeting breast cancer with novel organometallic complexes
P51	Ghannish Soogary	Novel ferrocenyl quinoline-benzimidazole molecular hybrids as antileishmanial agents
P52	Sandeep Kumar	Thermodynamics and computational study of the molecular interactions between water and imidazolium and pyrrolidinium based ionic liquids
P53	Muriel Mambanda	Adsorptive removal of dyes from an aqueous solution using UiO-66 metal organic framework
P54	Lishavia Mahabeer	Phytochemical screening of polyphenolic extracts from South African indigenous plants for inclusion in sunscreen products
P55	Rhoda Adegoke	Isotherm and kinetics studies on the adsorption of Zn^{2+} onto biochar/graphene oxide composites
P56	Zizipho Ngayeka	Synthesis and characterization of composite track-etched membranes for application in mine-waste waters

ABSTRACTS

Plenary 1: Organometallic-enhanced nanoelectronics and solar cells

Nicholas J. Long

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Keywords: ferrocene, organometallic, thermoelectrics, solar cells

The iconic organometallic 'sandwich' compound, ferrocene, has been studied for a myriad of different applications, spanning the fields of catalysis, materials chemistry and beyond, and even after 70 years, new uses for ferrocene are still being discovered. One particular field where ferrocene has gained interest is that of molecular electronics. Ferrocene has exceptionally well-defined redox chemistry that has seen it often included into molecular architectures, particularly involving metal-alkynes, as an electroactive component. These electronic properties, alongside the versatile substitution chemistry of ferrocene, has recently been exploited by us in developing highly efficient and stable perovskite solar cell devices. The presentation will cover our recent findings in utilising ferrocene in modern nanoelectronic devices (1, 2) and within the layer structure of perovskite solar cells (3).

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Plenary 2: Patterns in the engineering of smart functional materials for clean energy conversion

Emmanuel Iwuoha

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Keywords: Li-ion battery, Mn-ion supercapacitor, rare earth metal kesterites, solar cell

This presentation highlights studies on the designing of functional semiconductor materials with optimised electronic and electro-energetic properties for energy conversion applications [1], [2]. They include kesterite materials, i.e., $Cu_2ZnSn(S,Se)_4$ (CZTSSe), which have emerged as potential solar absorber materials [1], due to the earth abundance and sustainability of their constituent elements and their attainment of up to 12.6% power conversion efficiency in thin film solar cells. Kesterites possess excellent optical and semiconductive properties that make them suitable as p–type absorber materials in solar cells. However, they exhibit high open circuit voltage deficit due to antisite defects and secondary phase formation, resulting in poor device performance [2], thereby limiting their competiveness against Si-based solar cells. Novel transition metal- and inner-transition metal-substituted kesterites and oxychalcogenides were designed, synthesised and applied as potential solar absorbers with improved open circuit voltage and power conversion efficiency [3]. Manganese, which South Africa has 77% of its global abundance, is an important component of Li-ion battery materials. Its oxide ($LiMn_2O_4$), phosphate ($LiMnPO_4$) and silicate (Li_2MnSiO_4) are used as cathode materials in Li-ion batteries and supercapacitors, due to their high capacity and maximum energy density potentialities [4]. However, they have low electrical conductivity and poor structural stability caused by Jahn-Teller anisotropic lattice distortion of Mn^{3+} ions [5], [6]. Studies on the engineering of the chemical environment of the Mn-ion to reduce the Jahn-Teller effects will be presented. Also, the search for new types of active materials to be used as supercapacitor electrodes continues to be challenging. The presentation will include novel microwave-assisted synthesis of ruthenium antimony oxide (RuSbO) and ruthenium antimony oxide-graphene (RuSbO-G) composite materials [7]. Initial results on their cell specifications suggest their being promising electrode materials for asymmetric supercapacitor.

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Plenary 3: Dynamic Behaviour of Single Atomic Species and Nanoparticle Catalysts Revealed by In-Situ Transmission Electron Microscopy

Sarah J Haigh [a], Nick Clark [a], Sam Sullivan Allsop [a], Matthew Lindley [a], Rui Zhang [a], Yi-Chao Zou [a], Yi-Chi Wang [a], Rongsheng Cai [a], Thomas Slater [b] and Roman Gorbachev [a]*

[a] University of Manchester, National Graphene Institute, Department of Materials and Department of Physics and Astronomy, Manchester, United Kingdom. E-mail: sarah.haigh@manchester.ac.uk. [b] Cardiff University, School of Chemistry, Cardiff, United Kingdom.

Keywords: characterization, catalysts, MoS_2, gold, electron microscopy

Improving the selectivity and durability of metal single atom and nanoparticle catalysts requires accurate atomic scale characterisation methods. Scanning transmission electron microscopy (STEM) can directly image reveal the local elemental composition and atomic structure for these materials but the requirement for vacuum conditions can lead to unwanted changes in the structure of the catalysts. In-situ environmental cell electron microscopy overcomes this limitation to characterize these complex systems in environments that better represent those they experience in use. We have applied in-situ gas cell STEM to investigate how the catalyst morphology evolves for different catalyst compositions supported on titania prepared by wet impregnation synthesis. Both $AuPd/TiO_2$ and Co/TiO_2 industrial supported nanoparticle catalyst systems are compared. We also study how the starting structure and composition determines the evolution of industrial supported nanoparticle catalysts during activation heat treatment.[1] In-situ conventional gas cell STEM studies are complemented by ex-situ investigations which achieve higher spatial resolution, due to the absence of unwanted electron scattering produced by the SiN_x cell windows and gas layer.

We also report experiments using graphene liquid cells, which allow atomic resolution spatial resolution of solid catalysts surrounded by liquids. Our 2D heterostructure graphene liquid cell design enables functionality such as liquid-liquid mixing [2] and the study of atomic scale dynamics at a solid-liquid interfaces (Fig. 1).[3] While most STEM studies are often limited to 2D projections with limited spectroscopic information we have applied the single particle reconstruction (SPR) method, widely used in cryoEM imaging of biological systems, to is a valuable means to probe the 3D evolution of inorganic nanoparticles.[4,5] By averaging over many particles we show tomographic reconstructions at much lower electron dose than is required for conventional tilt series tomography, enabling imaging for active nanoparticle systems like PtNi; highly active catalysts towards the oxygen reduction reaction.[4,5] We show that this opens up the technique to allow 3D visualization at different time points during in a synthesis process or catalytic reaction.[6]

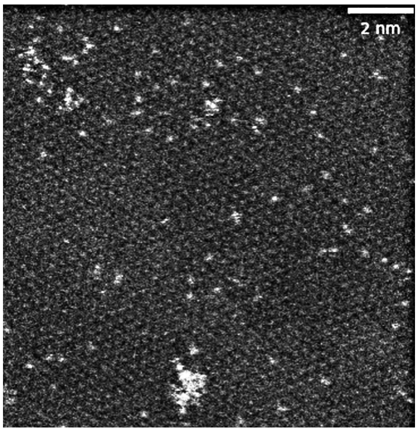

***Figure 1.** Atomic resolution annular dark field STEM image of Pt species on MoS_2 acquired inside a 2D heterostructure liquid cell (full video series in [3])*

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Keynote 1: Visible Light-Induced Bioorganometallic Chemistry: Illuminating New Frontiers

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Keywords: bioorganometallic chemistry, photochemistry, photopharmacology, malaria, cancer

One of the key areas of research in the fight against diseases is the creation of innovative therapeutic treatments. With the promising, nascent field of metal-based drug discovery, a number of platinum-based metallodrugs, such as the medically prescribed carboplatin and oxaliplatin, have been designed since the discovery of cisplatin [1,2].

Despite this, the same obstacles that restrict the use of cisplatin also impede the use of these metallodrugs: off-target effects, resistance development, and restricted range of activity [3,4]. Due to these constraints, the search for metallodrugs has shifted to other metals, with ruthenium leading the way. This is exemplified by a number of ruthenium-based complexes, such as NAMI-A, NKP-1339, and TLD1433, that have been clinically studied for the treatment of different tumours.

The treatment of diseases often involves traditional modalities which include immunotherapy, radiotherapy or chemotherapy. Certain traditional treatments are also associated with severe side effects. Consequently, researchers have focused on novel therapeutic treatment modalities and more recently, light-induced therapies have come to the fore. Among the studied treatment methods, photodynamic therapy (PDT) is one such modality already used in the clinic and has emerged as a promising complementary technique to chemotherapy [5,6].

In this presentation, the rational design and development of bioorganometallic compounds based on various pharmacophoric scaffolds of biological significance will be delineated. In particular, the versatility of several metal complexes in different light-based treatment modalities for malaria and cancer will be highlighted, notably against resistant forms of the *Plasmodium falciparum* parasite and HeLa cell lines respectively, and how nuanced structural alterations may influence the overall biological activity.

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Keynote 2: Probing the cytotoxicity of Pd(II) and Ru(II) metal complexes through the lenses of substitution kinetics and biomolecular interactions

Stephen O. Ojwach, Reinner O. Omondi, Nokwanda Tsaulwayo
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Keywords: Palladium, ruthenium, kinetics, biomolecular interactions, cytotoxicity

Despite the success of cisplatin in chemotherapy, its efficacy has been limited by severe side effects, drug resistance and poor pharmacokinetics [1]. This has germinated renewed interests in the design of superior alternative metal based chemotherapeutic agents [2]. Palladium and ruthenium complexes have recently emerged as suitable candidates to replace the well-established cisplatin [2]. Our research group has adopted a multidisciplinary approach to develop palladium and ruthenium metal complexes as potential anti-cancer agents as depicted in **Fig. 1** [3]. This encompasses understanding of the coordination chemistry and substitution kinetics of the complexes with the aim of regulating their resultant physical and physiological properties. Interactions of these complexes with small biomolecules such as DNA and BSA and molecular docking experiments are also performed to assist in the understanding of the experimental cytotoxicity trends. This lecture presents a systematic study on the coordination chemistry, ligand substitution kinetics and applications of palladium and ruthenium complexes of mixed-donor ligands as potential anti-cancer drugs.

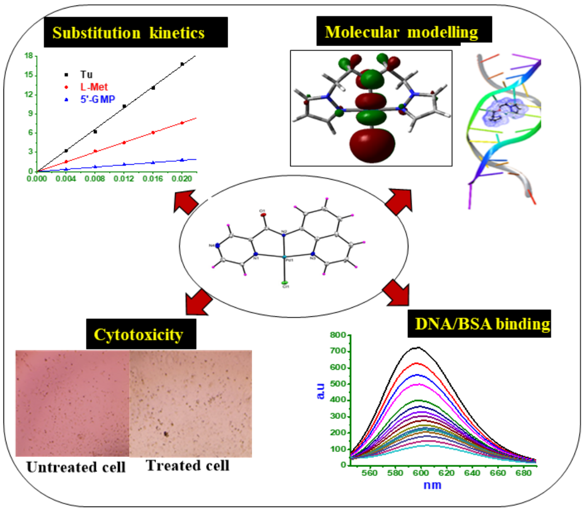

Fig. 1. Multidisciplinary approach to metallo-drug design and development

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Keynote 3: Molecular Insights into Inorganic Complexes using Computational Chemistry

Lydia Rhyman[a,b] *and Ponnadurai Ramasami*[a,b]

[a]Computational Chemistry Group, Department of Chemistry, Faculty of Science, University of Mauritius, Réduit, 80837, Mauritius, E-mail: lyd.rhyman@gmail.com. [b]Centre For Natural Product Research, Department of Chemical Sciences, University of Johannesburg, Doornfontein, Johannesburg, 2028, South Africa

Keywords: molecular, complexes, computational chemistry

Computational Chemistry involves the use of mathematical methods to solve chemistry and interdisciplinary problems. It has become useful to complement experimental research. It is more important as it provides molecular insights of chemical systems.

This talk will be based on our experience in the use of computational chemistry in our research on metal complexes, in particular, metal complexes of cyclen [1], ruthenium complexes [2] and complexes of f-block elements [3].

It is anticipated that this talk will be of incentives to use computational chemistry for research and will provide arena for collaboration [4].

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Keynote 4: Metal-driven co-selection of antibiotic resistance

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Keywords: Microbe-metal interactions, Environmental dimension of antibiotic resistance, Co-selection, Bacterial community assembly processes, Public health

Microbe-metal interactions play crucial roles for the biogeochemical cycling of metals and for planetary health. During the last two decades, the development of bacterial metal resistance in response to metal pollution has been increasingly linked to the co-development of antibiotic resistance (AR). Environmental metal-driven co-selection of antibiotic resistance constitutes a public health risk not presently accounted for within any existing regulatory risk assessment framework. In this keynote presentation, I will first introduce the global AR challenge facing mankind with a focus on its environmental dimension. I will then continue by reviewing the literature on metal-driven co-selection of antibiotic resistance for a predominantly non-microbiologist audience based on research conducted in my research group including a recently established curated database collating data on the effects of metals on all available antibiotic resistance-related endpoints. A decision tree based on data quality and environmental relevance was used to assess the evidence for causal relationships between metal exposure and the development of AR. High-quality studies were used to derive Minimal Co-Selective Concentrations for individual metals in soil, sediments, and water. I conclude that metal-driven co-selection of antibiotic resistance occurs in some metal-contaminated environments and that metals in some settings may confer stronger selective agents for development of antibiotic resistance than antibiotics do. However, the importance of metal-driven co-selection of AR for public health is still unknown due to the shortage of high-quality data for risk assessment and insufficient knowledge on the underlying co-selection mechanisms.

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Keynote 5: Nanocrystals: Breaking Boundaries in Alkaline Water Splitting

Nosipho Moloto, Tshwarela Kolokoto, Lineo Mxakaza, Zakhele Ndala, Siyabonga Nkabinde and Victor Mashindi

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Keywords: nanomaterials, water splitting, HER, OER

Hydrogen (H_2), while abundant on Earth, is primarily found within compounds like H_2O. To harness it for use as fuel, it needs to be separated into pure hydrogen, and various methods can achieve this, including water electrolysis. Hydrogen production's environmental impact and energy efficiency depend on the chosen method, which can involve fossil fuels, biomass, or clean processes like electrolysis. Electrolysis, particularly when coupled with photovoltaics for electricity, is considered a clean and renewable method of hydrogen production. The electrochemical processes of HER (Hydrogen Evolution Reaction) at the cathode and OER (Oxygen Evolution Reaction) at the anode are crucial in water splitting. Efficient catalysts are pivotal in promoting these reactions, ensuring a balanced and effective water-splitting process for sustainable hydrogen production. This report focuses on the synthesis and characterization of novel metal chalcogenides and mixed metal oxide nano-electrocatalysts for both HER and OER.

Keynote 6: Combined methods of preconcentration and degradation for removal of per- and polyfluoroalkyl substances (PFAS)

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Keywords: Per- and polyfluoroalkyl substances, concentration, advanced reduction process, defluorination

Per- and polyfluoroalkyl substances (PFAS) are synthetic organic chemicals, in which at least one or all hydrogen atoms attached to the carbon chain are replaced by fluorine. Due to the high strength of the C–F bond, PFAS exhibit high chemical and thermal resistance. The wide application of per- and polyfluoroalkyl substances has caused contamination of the environment worldwide. Human exposure to PFAS is related to various diseases, such as kidney cancer, testicular cancer, and thyroid disease.

Over the past few decades, several reduction and oxidation methods have been developed for the degradation of PFAS in water. One promising technique is the use of advanced reduction processes (ARPs) with a UV/sulfite system, which have shown high degradation and defluorination efficiency for PFAS due to the generation of highly reactive radicals, i.e., hydrated electrons [1] [2]. For example, the concentration of perfluorooctanoic acid was below the detection limit after 1 h (at pH 10) while 89% defluorination was achieved after 24 h [3]. Short-chain perfluorinated carboxylic acids and hydrogen substituted compounds were detected, which indicates chain-shortening and H/F change reactions. However, the typical concentration of PFAS reported in contaminated water is usually too low (ng/L to µg/L) to be directly treated using a UV/sulfite system, making it uneconomic in most situations. Therefore, pre-treatment methods that concentrate PFAS are necessary before applying the UV/sulfite system. This presentation aims to discuss the challenge of low PFAS concentrations in contaminated waters as well as outlining solutions to overcome this challenge. Specifically, the combination of ion exchange/desorption and reductive UV/sulfite degradation to eliminate PFAS is explored.

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Keynote 7: The role of noncovalent interactions in the properties of porous compounds

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Keywords: noncovalent interactions, computational chemistry, structure

Noncovalent interactions play a fundamentally important role in the properties of solid materials. As an example, guests are taken up into the host framework of porous materials as a result of the interactions between these species, while the manner in which they interact has an influence on the sorption ability of the porous material. In this work, calculations on a range of porous frameworks allow us to explain the role that noncovalent interactions play in the sorption properties of these compounds.

For instance, a member of the family of trianglimines, a triangular-shaped molecule that crystallises to create nano-sized channels running the length of the crystals, interacts strongly with water molecules resulting in a colour change [1]. Calculations show that the colour change is a result of ketoenamine tautomerism that occurs concomitantly with rapid uptake of water at relative humidities above 55%. Surprisingly, if the humidity is reduced to below 55% a front of yellow colour is observed indicating there is a similar fast release of the water out of the crystal, even down to temperatures as low as –70 °C. Metropolis Monte Carlo studies confirm that water molecules can diffuse through the channels at these low temperatures.

It has also been shown that the origin of anomalous sorption isotherms are the result of interactions between acetylene [2] or carbon dioxide [2,3] and the host frameworks, as well as interactions between guests. Similarly, noncovalent interactions are responsible for the change in colour along an hourglass pattern of a crystalline porous compound during sorption of particular solvents. Calculations show that the origin of this effect is that the channels in the porous framework are anisotropic, allowing sorption only from particular faces [4].

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Keynote 8: Recent progress in nanotechnology van der Waals heterostructures

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Keywords: 2D materials, van der Waals heterostructures

In the last years, a novel field has emerged which deals with structures and devices assembled layer-by-layer from various atomically-thin (2D) crystals. These new multi-layer structures have proved to be extremely versatile, showing exceptional electronic and optical properties, new physics and new functionality. This is mostly due to the fact that each atomic layer can be chosen among many different materials including metals, semiconductors, superconductors or even topological insulators. In this talk I will review recent progress and challenges in the field of van der Waals heterostructures.

I will cover the development of electronic devices based on 2D materials, starting from the early age of the field and discussing technological milestones in its development. Advantages and challenges of mechanical stack assembly from exfoliated or large scale grown 2D materials will be compared to that of directly grown heterostructures. Air sensitivity of more exotic 2D materials will be discussed and subsequent attempts to perform nanofabrication of such structures in inert gasses and vacuum. I will then review new properties arising from the interface between 2D materials, for instance graphene and moiré superlattices and associated phenomena. I will end the talk discussing the field development and current limiting factors, such as crystal quality, contamination and environmental sensitivity of 2D materials.

Keynote 9: Cushioning the global transition to clean energy through sustainable sourcing and processing of fuel oils

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Keywords: fossil fuels, biofuels, adsorptive pre-treatment, hydroprocessing.

Within the 'Just Transition' in the energy sector of South Africa, the use of fossil fuels remains high in the envisaged energy mix. Reliance on crude oil and coal, and a slow transition to green and renewable sources of fuel is problematic making it imperative to develop and strengthen strategies for the sustainable use of fossil fuels for the current and mid-term future needs [1]. Herein, we propose strategies for blending the coal fines and biomass to produce bio-crudes as a possible measure towards sustainability [2]. We also present chemical strategies for improving the processing of these oils considering their higher concentrations of heteroatoms (nitrogen, oxygen and sulfur), aromatics and long chain paraffins compared to straight-run oil fractions. We demonstrated the significance of pre-treating such feedstocks to remove the nitrogen and oxygen compounds using coordination polymers and comparative hydroprocessing results showed the potential for hydroprocessing these feedstocks using mild conditions and conventional catalysts. The mechanism of application of the novel adsorption process was fully studied using a range of techniques such as TGA, FTIR and XRD. An overview for incorporating this strategy in improving conventional hydroprocessing is presented in Figure 1.

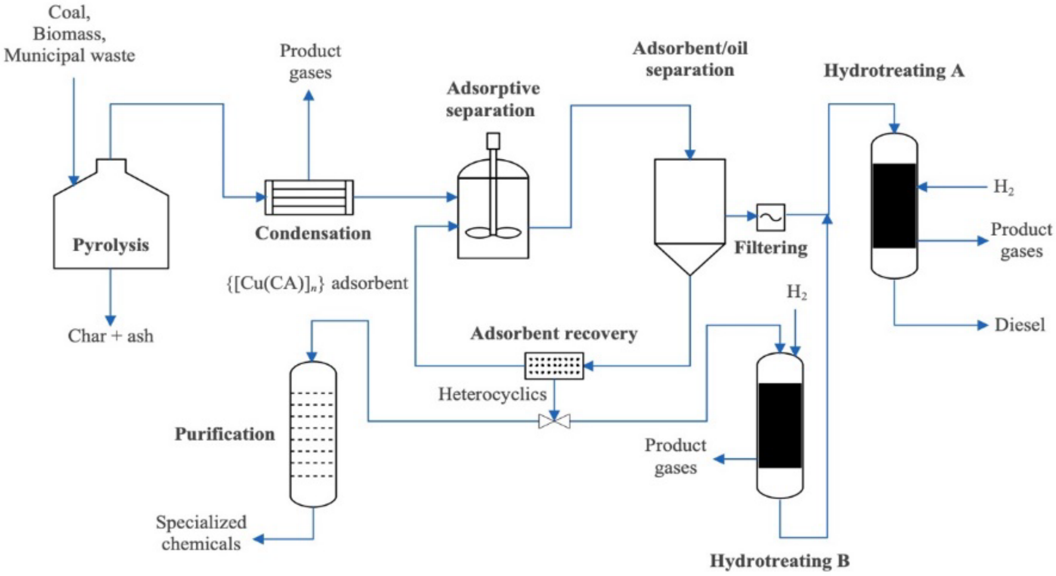

Figure 1: A process flow diagram for beneficiation of fossil or biomass based solid fuels to liquid fuels and chemicals.

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Keynote 10: Metal-organic precursor-derived functional nanomaterials for energy generation and storage applications

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Keywords: Metal-organic precursors, HER, OER, ORR, Supercapacitance

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Currently, 80 % of our energy needs are met by non-renewable fossil fuels (i.e., oil and coal), which are depleting at a faster rate. In addition, fossil fuels are the major cause of environmental pollution. Therefore, renewable and environmentally friendly energy sources are highly required. Electrocatalytic reactions for energy generation, such as oxygen reduction and hydrogen evolution and oxygen evolution via water splitting are considered cost-effective, sustainable and green alternatives to fossil fuels. However, water is thermodynamically highly stable, and obtaining hydrogen by splitting water is a challenge. Similarly, ORR can occur either by a 2-electron pathway leading to the formation of H_2O_2 or by a 4-electron mechanism to generate water and selectivity is required. Likewise, as a step towards the implementation of sustainable energy development strategies, research on the design of high-performance energy storage systems, such as supercapacitors is gathering renewed momentum.

Some important pre-requisites for developing promising catalysts are that they must be composed of earth-abundant, eco-friendly and cost-effective materials. In addition, they should show high electrocatalytic activity and stability under desired reaction conditions. For supercapacitors, they should have a high energy density as well as high power density.

Synthesis of such materials with shape, size and precise compositional control is highly challenging. We have demonstrated that metal-organic precursors are advantageous in controlling phase and composition due to the presence of pre-formed bonds between metal and the chalcogenide atoms [1-2]. They are usually stable and equally suitable for the preparation of nanomaterials as well as the deposition of thin films. The properties of metal-organic precursors can be tuned by modifying the backbone structure of the ligands. Depending on the synthetic route and targeted materials, careful designing and selection of the precursor is required. The focus of the talk will be the designing of suitable precursors, their use in the preparation of complex functional nanomaterials via different synthetic routes, and strategies to bolster their performance for ORR, HER, OER and supercapacitance.

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Keynote 11: Digital manufacturing meets catalysis: some examples of 3D printing in chemistry

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Keywords: 3D printing, catalysis, flow chemistry, robotics.

Digital manufacturing such as 3D printing, laser cutting and CNC machining are currently a very hot topic worldwide. Due to the Open Source Hardware revolution, which started in the early 2000s, a large amount of low cost hardware can be produced locally. By combining a range of Open Source Hardware items such as 3D printers, Arduino electronics, etc, it is possible to produce the necessary hardware for a low-cost laboratory [1]. We started investigating the use of 3D printing in chemistry around 2017 and will report some of the uses of digital manufacturing in this presentation.

As inorganic chemists with a focus on catalysis, we will present our work on a number of research topics related to digital manufacturing. Here, we will present our work on home-built flow chemistry [2], including the use of digitally manufactured monoliths for catalysis [3]. We will also describe our work on 'catalytic stirrer bars' and 'catalytic flow chips'. These developments are low-cost and can be implemented in any laboratory.

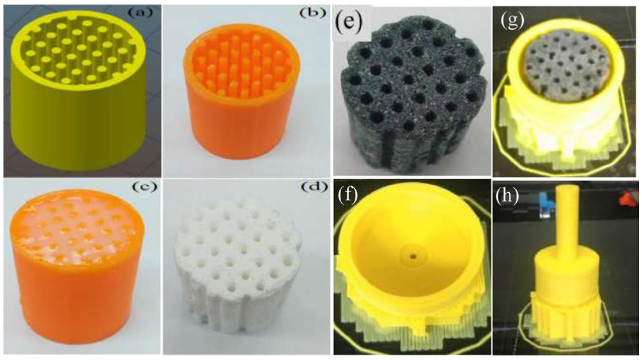

Figure 1: (a) 3-*D* rendered design of the sacrificial templates (b) 3-D printed sacrificial templates (c) 3-D printed sacrificial templates containing the alumina paste (d) Alumina monolith (MNT) (e) Pd/MNT (f) half printed reactor (g) Incorporation of the catalyst (h) fully printed reactor containing the Pd/MNT catalyst.

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Invited 1: Structural chemistry of cyanoximes

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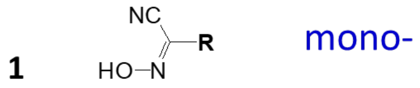
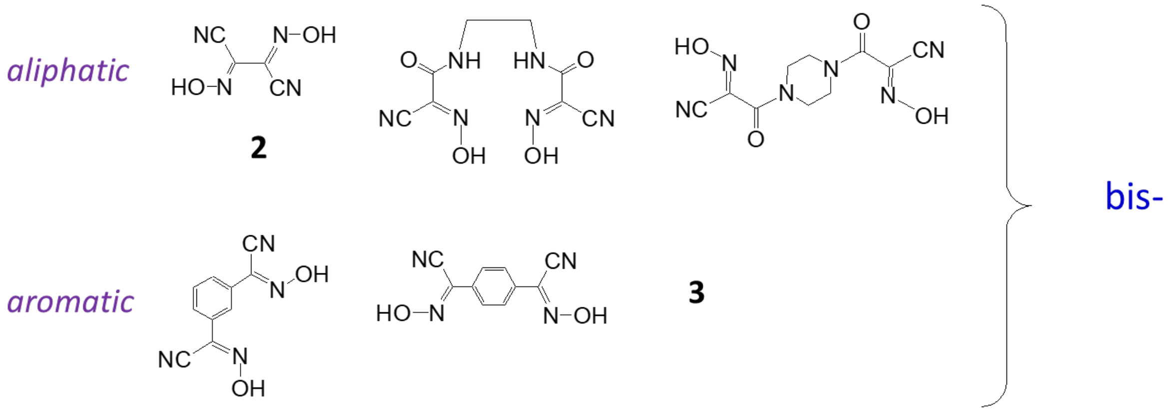
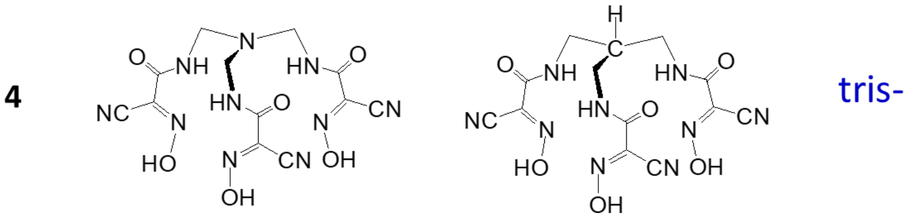
Keywords: cyanoximes, structures, properties, applications

During the last three decades research chemistry of the new subclass of organic ligands – cyanoximes – that have general formula NC-C(=NOH)-R where R is an electron-withdrawing group has been developed. Presence of CN-group makes cyanoximes ~10,000 more acidic and better ligands than other known oximes. With 38 different R groups the most abundant is the family of mono-cyanoximes **1** (below), followed by bis-cyanoximes **2**,**3** that include aromatic and aliphatic spacers, and lately tris-cyanoxime **4** - a tripod - was obtained and characterized. Therefore, a large library of new low-molecular weigh organic compounds with the variety of different properties was created.







These simple low molecular weight organic molecules represent series of new excellent ampolydentate ligands for coordination chemistry: new types of molecular Legos. Both un-complexed ligands, their Na^+ and K^+ salts and other metal complexes (Ni, Ag, Sb, Pd, Pt) show a large spectrum of biological activity from antimicrobial and growth regulation in plants to significant *in vitro* and *in vivo* cytotoxicity against human cancers. Currently 45 cyanoximes are known, and there were more than two hundred cyanoxime complexes synthesized and studied using X-ray analysis. Stereochemistry of cyanoximes ligands, their most interesting metal- and organometallic compounds are reviewed, while numerous *practical applications will be presented and discussed* with interested parties after the talk.

Invited 2: Novel nanocomposites and mixed oxide material as recyclable catalysts and other applications

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Keywords: Green Chemistry; Mixed oxides; Heterogeneous catalysts; Value added conversions.

Adoption of green protocols is vital for a sustainable environment and development. Given the stringent environmental legislation and associated obligations, the chemical industry encourages procedures that adhere to green principles. Enhanced selectivity, atom economy, and energy efficiency in various chemical reactions are attainable by employing appropriate materials as catalysts. In recent years, the fabrication of novel nanocomposites involving biomaterials and as supports has received ample attention. The mixed oxides and their composites offer multiple advantages, including excellent thermal stability, crystallinity and shape selectivity. The recyclability of the materials makes their usage in the synthetic protocols more attractive.

Based on the experiences of our research group in developing varied heterogeneous materials and nanocomposites, their competence as efficient catalysts in synthesising various novel bioactive heterocyclic moieties by multicomponent approach under green conditions will be described.

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Invited 3: Photocatalytic green hydrogen production using semiconductor heterojunctions

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Keywords: Green Hydrogen, Photocatalysis, semiconductor heterojunctions

A clean and sustainable energy source is required to address the increase of global energy demand and the carbon-related environmental issues. Semiconductor-based photocatalysis has received tremendous attention because of its potential for solving current energy and environmental problems. In a semiconductor photocatalytic system, photo–induced electron-hole pairs are produced when a photocatalyst is illuminated by light with energies larger than that of its band gap. These photo-excited charge carriers can either recombine or migrate to the surface of the semiconductor, where they can be involved in redox processes. The photocatalytic efficiency depends on the number of charge carriers and the lifetime of the electron hole pairs generated by the photoexcitation. High recombination rate of photo-excited charge carriers and limited efficiency under visible light irradiation are the two limiting factors in the development of efficient semiconductor-based photocatalysts.

We present the design, preparation, characterization, and photocatalytic performance of several semiconductor heterojunctions used to enhance green hydrogen production using visible light. The study of these systems demonstrates that the design and preparation of heterojunctions with proper band gaps and relative band positions can facilitate charge separation/migration and decrease the charge recombination rate, thus enhancing the photocatalytic efficiency in visible light. Based on observed activity, band positions calculations, and photoluminescence data, a mechanism for the enhanced photocatalytic activity is proposed and discussed [1].

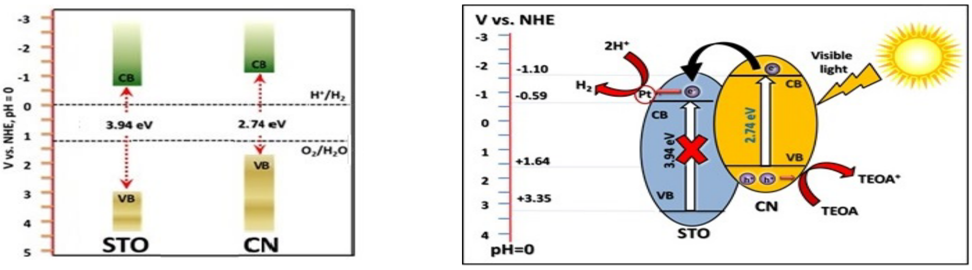

Fig. 1. Schematic diagram showing a semiconductor heterojunction made of one visible light active and UV light only active component.

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Invited 4: Understanding the photochemistry of perovskites for photovoltaics

Matthew Lloyd Davies[ab]*, Emmanuel V. Péan*[a]*, Rodrigo García Rodríguez*[a]*, Pavlina Kalyva*[a] *and Karen Valadez Villalobos*[a]*.*

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Keywords: Perovskites, photoluminescence, stability, sustainability.

Thanks to their high absorption coefficient and ideal band-gap [1], lead halide perovskite materials are good candidates for the next generation of solar cells with an impressive certified power conversion efficiency of >26% [2]. However, the development of perovskite based solar cells is impeded by obstacles including degradation of the perovskite layer by light, oxygen, and moisture. Photoluminescence (PL) is a measure of photoexcited carrier radiative recombination and is thus a great tool for studying charge carrier processes in solar cells as the later operates through the absorption of light. However, measuring the steady state and time-resolved photoluminescence (PL) of perovskite thin-films is not as straightforward as initially thought, highlighting the sometimes-surprising nature of these materials. [3-5] Here, we discuss our utilisation of PL studies to understand the stability and performance of perovskite materials; particular in assessing alterations to manufacture and materials to improve the sustainability of perovskite solar cells (e.g the use of carbon electrodes as alternatives to gold). This is complimented via XRD and SEM analysis to understand the effect of material substitutions on the morphology and uniformity as well as photovoltaic device performance. We will discuss the work of The Applied Photochemistry Group at the SPECIFIC Innovation and Knowledge Centre, Swansea University, which aims to develop an understanding of the photostability and photochemistry of materials and devices to advance sustainable perovskite photovoltaics lab-scale to production scale manufacture.

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Oral 1: Synthesis, characterisation, DNA binding and cytotoxic studies of novel phenanthroline-derived oxovanadium(IV) complexes

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Keywords: Oxovanadium(IV), Schiff base, crystal structure, DNA binding, dpq.

Current pharmaceutical research aims to develop more effective and less toxic anticancer drugs than cisplatin and related second-generation anticancer platinum drugs using coordination compounds of transition metals such as vanadium.[1-3] In this work, oxovanadium(IV) has been selected as the metal centre for the design of novel anticancer agents. 1,10-Phenanthroline (PHEN) and dipyrido[3,2-d:2',3'-f]quinoxaline (DPQ) were chosen as the co-ligands in the heteroleptic complexes based on these ligand's ability to bind to DNA.[4] The syntheses, characterisation, stability, DNA binding, DNA cleavage activity and cytotoxicity of novel complexes of the type [VO(ONO)(DPQ)] (**1,2**) and [VO(ONN)(NN)]PF_6 where NN = PHEN (**3,4**) and DPQ (**5,6**), as shown in Figure 1 (a,b), are reported. Complexes **2-4** have been structurally characterised by single-crystal X-ray diffraction. The solid-state structures reveal a six-coordinate VN_3O_3 (for complex **2**) or VN_4O_2 (for complexes **3** and **4**) coordination geometry with the Schiff Base ligand coordinated in a tridentate ONO- or ONN- fashion to the oxovanadium(IV) centre and the N_2-donor (PHEN or DPQ) *trans* to the vanadyl oxo-group. DNA binding studies were carried out on the complexes using absorption titrations and emission spectroscopy, gel electrophoresis, micro-viscometry and molecular docking simulations (Figure 1(c)). The DPQ complexes show good binding propensity to calf thymus DNA, binding in partial intercalative and groove-binding modes. Complex **1** could oxidatively cleave plasmid DNA in the presence of H_2O_2 by producing hydroxyl radicals. Complexes **5** and **6** were able to cleave DNA *via* a singlet oxygen pathway. Complexes **1-6** are cytotoxic against the triple-negative breast cancer MDA-MB231 and neuroblastoma SH-SY5Y tumour cell lines. Complexes **3-6** are cytotoxic towards the HeLa cervical cancer cell line. Complex **5** is significantly more toxic to the carcinoma cell lines than the healthy renal cell line HEK293.

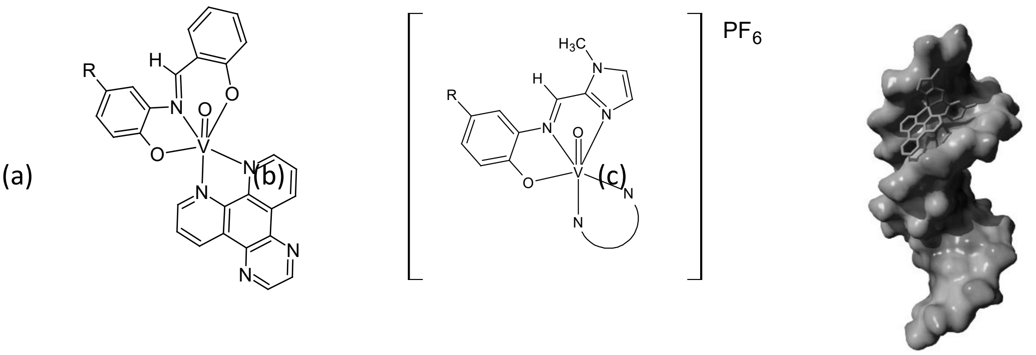

Figure 1: (a) Structures of complexes [VO(ONO)(DPQ)] (R = CH_3 (**1**), $(CH_3)_3$ (**2**) and (b) [VO(ONN)(NN)]PF_6 (R = CH_3 (**3,5**), $(CH_3)_3$ (**4,6**); NN = PHEN (**3,4**), DPQ (**5,6**). (c) Complex **5** docked into minor-groove of B-DNA.

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Oral 2: Solid-state crystalline structures of baclofen

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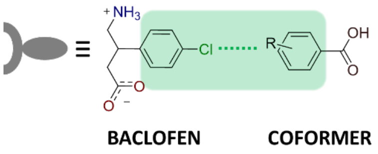
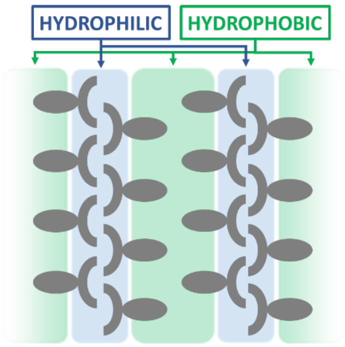
Keywords: baclofen, polymorphism, multicomponent crystals

Baclofen, *(RS)*-4-amino-3-(4-chlorophenyl)butanoic acid, is a slightly water-soluble hydrophobic γ-amino acid and primarily used as a muscle relaxant. Recently, it was repurposed for the treatment of early-onset alcoholism, which is an increasing problem in young adults and adolescents. Baclofen has low solubility that influences its efficacy; thus, exploring the solid-state structures of the drug offers opportunities to enhance its properties. Our research group has been interested in the supramolecular modification of baclofen since 2014. Firstly, we aimed to improve the properties of the drug by forming multicomponent crystals. Baclofen was successfully cocrystallised with selected mono- and dicarboxylic acids, yielding four molecular salts. The packing of the crystals (with the exception of the maleate salt) comprises hydrogen-bonded layers formed by the polar heads and the carboxylic groups of the coformers, which alternate with hydrophobic aromatic layers. It was observed that there is some dependence between the percentage of O···H interactions and the melting points of the crystals. [1]

Based on these observations, we speculated that using acidic and basic coformers of increasing size and varying polarity would preserve the crystal's general layered structure while enabling fine-tuning the intermolecular interactions in the aromatic layer. Thus, we extended the landscape of the solid-state structure of baclofen by cocrystallising it with halogenated aromatic carboxylic acids and nitrogen-containing heterocycles. [2] A comparative crystal packing study showed that the most common packing motif of the multicomponent crystals is the formation of the hydrogen-bonded baclofen chains in a head-to-tail manner with fine-tuned aromatic layers.

This strategy was extended by using coformers with nitro functional groups that form directional but weak interactions in the hydrophobic layer. [3] The nitro and the chloro groups act as weak hydrogen bond acceptors and would not disrupt the hydrogen bonding in the hydrophilic layer; instead, the nitro group directs the packing in the hydrophobic layer, so the overall packing of alternating hydrophilic and hydrophobic layers is retained.





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Oral 3: Pd-catalyzed cross-couplings in the synthesis of non-canonical amino acids for the use in hydrogelators

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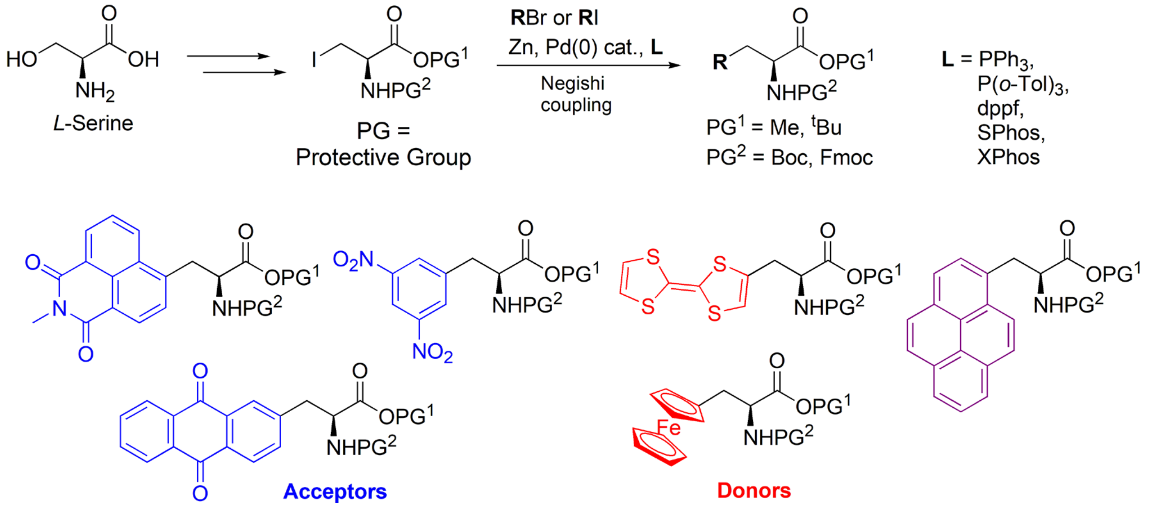
Keywords: cross-coupling reactions, non-canonical amino acids, peptides, hydrogelators

Only 22 natural α-amino acids appear in the genetic code of all life and in proteins, limiting the variation of possible peptides structures that can be synthesized from abundant naturally-derived starting materials. In recent years, the synthesis of amino acid with substituents not encountered in nature (non-canonical, or unnatural, amino acids) has attracted significant research efforts [1].

Employing proteogenic amino acid *L*-serine **1** as starting material we have synthesized various non-canonical amino acids. As the key transformation, we used the Pd-catalysed Negishi coupling of protected 3-iodo-*L*-alanine derivatives [2], prepared from *L*-serine in three synthetic steps. Amino acid derivatives with acceptor, donor, and fluorescent polyaromatic hydrocarbon residues have been synthesized using this synthetic approach. Whereas most of the coupling reactions proceeded under the "common" Negishi reaction conditions with good yields, for electron-reach substrates extensive optimization was required.

The novel donor- and acceptor-modified amino acids were used to synthesize and test the hexapeptide sequences forming the fibre-based hydrogels [3] for their use as drug delivery systems with prolonged drug-release capability. The presence of redox-active groups, such as tetrathiafulvalenes [4], in peptide sequence may enable the electron transport, and the future application of such redox-active nano-structured peptide-based materials in organic electronics can be envisaged.



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Oral 4: Enhanced HDS and HYD activity of sulfide Co-ligand/Mo catalyst supported on γ-alumina

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Keywords: Hydrodesulfurization, Hydrogenation, Co-L/Mo Complexes, supported catalysts

Deep hydrodesulfurization (HDS) of fuel oils continues to attract research interest due to environmental-driven regulations which limit its sulfur content in fuel to 10–15 ppm [1]. In a recent study conducted at Nelson Mandela University to improve HDS catalysts, Co-LMo catalysts using cobalt(II) nitrate and ammonium heptamolybdate in the presence of ligands-ethylenediaminetetraacetic acid (EDTA), citric acid (CA), and acetic acid (AA) were prepared on γ-Al_2O_3. SC-XRD of unsupported Co-LMo (L= EDTA) confirmed Co coordination with EDTA in a hepta coordinated–(N_2O_5) environment (Figure 1). The study on the effect of L (EDTA, CA and AA) on Co/Co + Mo) 0.3 in Co-LMo/Al_2O_3 catalysts on HDS pathways of dibenzothiophene (DBT) indicated that ligand exhibited significant influence on HDS and hydrogenation (HYD) pathway but showed no influence on direct desulfurization (DDS) pathway. Generally, ligands exhibited optimum promotion effect of Co for HDS by HYD route due to increased dispersion of MoO_3. H_2-TPR characterization indicated that the addition of ligand reduces the interaction between Al_2O_3 support and the active metals and led to the formation of the easily reduced Mo species (MoS_2), which formed more active sites [2], [3]. Enhancement of HDS rates was in the following order: CoMo-CA/γ-Al_2O_3 (98%)> CoMo-AA/γ-Al_2O_3 (94%) > CoMo-EDTA/γ-Al_2O_3 (90%) > CoMo/γ-Al_2O_3 (43%). These studies have contributed to increasing the understanding of catalyst design for achieving improved performance of deep HDS catalysis.

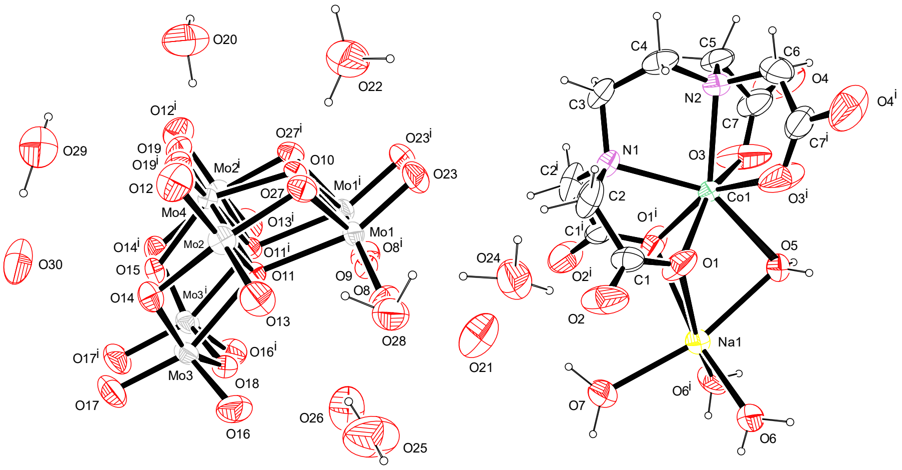

Figure 1. ORTEP diagram of Co-L(EDTA)/Mo with ellipsoids drawn at 50% probability level. Symmetry elements: (i) 1-x, +y, +z. Selected symmetry generated disorder of the EDTA ligand omitted for clarity.

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Oral 5: Visible light active metal supported TiO_2/C nanohybrids for photocatalytic removal of organic compounds in water

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Keywords: TiO_2, Photocatalysis, Carbon nanotubes, sol-gel, photoefficiency

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The urgent need for effective solutions to combat environmental pollution has led to intensified research efforts focused on developing advanced nanomaterials with enhanced capabilities. Among these, the hybridization of nanocarbons with semiconductor materials stands out as a promising strategy for designing next-generation photocatalytic materials for water purification. Titanium dioxide (TiO_2) photocatalysis, particularly the generation of highly reactive hydroxyl radicals (OH•) from TiO_2 valence band holes, has been a cornerstone in this area of study.Carbon-based materials, including carbon nanotubes (CNTs), fullerenes, activated carbon, graphene, carbon nanodots, carbon nanospheres, and carbon nanofibers (CNF), have emerged as valuable supports for TiO_2, offering various advantages such as retardation of electron-hole recombination, increased pollutant adsorptivity, efficient dispersion of semiconductors, and enhanced absorption in the visible light region, thereby acting as photosensitizers for TiO_2.Synthesis techniques for these nanohybrids can be ex-situ or in-situ, involving covalent or non-covalent bonding, with common fabrication protocols including chemical reduction, grafting, sol-gel, and gas phase deposition. Despite significant progress, opportunities remain for the development of novel synthesis protocols to fabricate TiO_2/carbon nanohybrids with diverse morphologies, leveraging the metallic or semiconducting nature of the nanocarbons to dictate potential transfer pathways within the hybrid components.

A deeper understanding of the physical and chemical properties of these nanohybrids promises further advancements in improving quantum yields for pollutant degradation. Comparison of different carbon allotropes in TiO_2 nanohybrids offers insights into their specific contributions, given their similar electronic and structural properties. In addition to carbon-based nanohybrids, the photocatalytic activity of TiO_2 can be enhanced through metal doping or deposition, with platinum group metals (Pt, Pd, Ir) forming Schottky barriers at the metal/TiO_2 interface to prevent electron-hole recombination, thus increasing photocatalytic efficiency. While most studies have focused on using UV radiation for photocatalytic experiments, the development of hybrid photocatalytic materials that can utilize solar light as an irradiation source holds promise for providing potable water solutions, especially for rural and disadvantaged communities.

In this study, Pd-supported TiO_2/MWCNTs, TiO_2/CNF, TiO_2/CB, and TiO_2/MWCNT-CNF nanohybrids synthesized through a sol-gel-derived organically modified silicate binder method will be evaluated for their visible light photocatalytic performance in degrading organic compounds in water. Leveraging the synergistic properties of TiO2-MWCNT and TiO_2-CNF, the Pd-supported TiO_2/MWCNT-CNF nanohybrid is expected to exhibit enhanced photoefficiency, contributing to the development of sustainable water purification technologies.

Oral 6: Dithiophosphonates as versatile precursors to the formation of nickel sulphides and phosphides towards water splitting

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Keywords: dithiophosphonates, nickel phosphides, nickel sulphides, water splitting

Interest in cost-effective and easily available materials employable as catalysts in water splitting is growing [1]. This is because of the current quest to move from a fossil fuel-based economy to a greener sustainable one [2]. Single-source precursors are a straightforward route to the formation of these desired nanomaterials [3]. We report the synthesis of the phosphorus and sulphur-containing dithiophosphonate complexes of the type $[Ni\{S_2P(OR)(4\text{-}C_6H_4OMe)\}_2]$ [Me = Methyl; R = H (**1**), C_3H_7 (**2**)], $[Ni\{S_2P(OR)(4\text{-}C_6H_4OEt\}_2]$ [Et = Ethyl; R = $(C_6H_5)_2CH$ (**3**)], $[Co\{S_2P(OC_4H_9)(4\text{-}CH_3OC_6H_4)\}_3]$ (**4**) and $[Fe\{S_2P(OH)(4\text{-}CH_3OC_6H_4)\}_3]$ (**5**) their structures confirmed by single crystal X-ray studies. The nickel atoms in the complexes adopted a square planar geometry as expected. The decomposition of complexes **1-3** in the presence of trioctylphosphine yielded nickel phosphides while the sulphides were formed in the presence of oleylamaine. Nickel phosphide doping with transition metals was also shown employing complexes **4** and **5**. Furthermore, the preparation of nickel phosphides and doping via the solvent-less route was shown. It is interesting to note that the formation of nickel phosphides through the solvent-less route is rare. Dithiophosphonates are also potential precursors for the formation of metal selenides and the ferrocenyl analogues which can be precursors to the formation of ternary systems. The electrocatalytic performance of prepared sulphides and phosphides in generating hydrogen and oxygen via water splitting was also examined with excellent performance.

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Oral 7: Waste to value: How can we effectively convert waste into useful materials?

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Keywords: Waste, Pollution

With the increased industrialization, urban and population growth, environmental pollution has become the major contributor to global warming and climate change, a greatest problem facing humanity [1]. The most common pollutants of the environment include plastics/low-density polyethylene (LDPE) from retail industries, coal fly ash (CFA) from mining industries, biomass from agriculture and waste cooking oil waste (WCO) from food manufacturing businesses. While there are some measures in place to try and minimize the waste (for example recycling of plastic and conversion of waste oil to biofuel), the rate of waste generation overwhelms its recyclability [2], and as such this waste still finds its way to the land, air and water, which is a direct threat to the ecosystems and species. It is thus crucial to re-direct waste and convert it into other useful materials of value.

This study demonstrates how waste such as LDPE, CFA, biomass and WCO could be effectively converted to useful materials for various applications such as water purification systems, engineering materials and catalyst support materials for energy applications. Our data shows that waste-derived materials produce similar results, to those produced using pure starting materials. This offers a cheap, sustainable way to produce high-quality materials, thus putting value to waste, while combating pollution for a sustainable environment and health.

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Oral 8: Synthesis and properties of metal-organic frameworks derived from waste feedstock

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Keywords: Metal-organic frameworks, polyethylene terephthalate, waste valorization

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Metal-organic frameworks (MOFs) are crystalline coordination polymers arising from the self-assembly of organic linkers and central metal ions or clusters. MOFs have continued to receive intense interest for a variety of applications due to their remarkable properties. They possess low weight, exceptionally high surface areas, large free volumes, and tunable pore sizes and functionalities, which make them very attractive for various applications such as sensors, gas adsorption and separation, catalysis, drug delivery, renewable energy and environmental applications, and magnetic and optical devices. These properties set MOFs apart from other porous materials like zeolites and carbon nanostructures. However, the consumption of large volumes of harmful solvents, high temperature and long durations needed for MOF synthesis, and the high cost of precursors are hampering the large-scale production of MOFs for practical applications. Therefore, sustainable approaches to MOF synthesis are being sought. This presentation will focus on our work on the synthesis of MOFs from waste precursors in an effort to lessen the burden on the environment and lower the cost associated with MOF synthesis. The utilization of waste metal sources such as eggshells, aluminium beverage cans and acid mine drainage waters will be discussed. Furthermore, the use of polyethylene terephthalate waste bottles as a source for organic linker will be presented. The properties of the MOFs will be evaluated. The work demonstrates our efforts towards more sustainable synthesis of MOFs and thus contributing towards advancement of their large-scale production for various applications.

Oral 9: Construction of S–Scheme 0D/3D $Cd_{0.5}Zn_{0.5}S/CeO_2$ heterojunction for the degradation of Cr(VI) and Antibiotics

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Keywords: S–Scheme; wastewater; antibiotics; heterojunction; Cr(VI) reduction

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A highly efficient $Cd_{0.5}Zn_{0.5}S/CeO_2$ heterojunction photocatalyst was developed through a facile solvothermal process for the photocatalytic reduction and oxidation of Cr(VI) and ciprofloxacin, respectively. The synthesized CZS/CeO_2 heterojunction exhibited higher photocatalytic activity than that of pristine CZS and CeO_2. In the presence of visible light, the optimal CZS/CeO_2 composite demonstrated its highest catalytic performance, achieving complete removal of Cr(VI) within 30 minutes with a catalyst dosage of 30mg. Additionally, it exhibited an 86% removal of ciprofloxacin (CIP) in the same timeframe and with the same catalyst dosage. This notable efficacy was observed at a molar ratio of 1:1. The improved photocatalytic activity of the composite is attributed to the enhanced charge carrier transport and separation of the catalyst. The S-scheme charge transfer mechanism was shown to be responsible for the enhanced charge carrier separation and consequently, the improved photocatalytic activity. Furthermore, the CZS/CeO_2 heterojunction also showed improved photocurrent intensity and reduced charge transfer resistance as compared to pristine materials (CeO_2 and CZS). The primary reactive species responsible for CIP degradation were identified as photo-generated h^+, $OH^\bullet$ and $\bullet O^{2-}$. Additionally, e^- was found to be mainly liable for Cr (VI) photoreduction. Furthermore, we propose a plausible photocatalytic reaction pathway for the elimination of both TC and Cr(VI). More importantly, this study clearly shows that CZS/CeO_2 heterojunction holds great promise for applications in wastewater treatment techniques.

Oral 10: Thermochromic aluminium-based fumarate MOF and its kinetic adsorption for nitrogen containing compounds

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Keywords: porous, adsorption, kinetics, colour change, contaminants

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Metal-organic frameworks (MOFs) have been studied for their interesting features that include large surface area and high porosity for potential applications. These porous structures are attractive in solid-state investigation for adsorption, catalysis, magnetism, and sensing. MOFs are characterized by different responsiveness against external stimuli such as solvent and temperature. The frameworks can collapse or stay stable depending on the strength of polarity of guest molecules and the nature of the framework. Aluminium-based MOFs are among frameworks that are highly stable towards strong polar guest molecules such as H_2O. The environment or water in general, may be contaminated by nitrogen containing compounds such as NH_4^+, NO_3^-, NO_2^-, and NH_3. These contaminants need to be removed for a sustainable environment. However, few studies reported on the use of aluminium-MOFs for the adsorption of nitrogen contaminants. This work has synthesized aluminium-fumarate MOF using aluminium extracted from waste (beverage cans) and fumaric acid as ligand, for adsorption of dimethylformamide (DMF), H_2O, and nitrogen containing compounds. The resulting MOF was activated at different temperatures to afford different phases characterized by color change from white to yellow. The latter activated form was tested for absorption of ammonia, H_2O, and DMF which was monitored by thermal gravimetric analysis (TGA) and powder X-ray diffraction (PXRD). Kinetic sorption for removal of both ammonia and water was computed to compare corresponding activation energies. We also have an ongoing study of this MOF extended for the removal of NH_4^+ and NO_3^- from water at different pHs. This will draw a conclusion at what pH aluminium-fumarate MOF can effectively remove both contaminants. Therefore, the use of aluminium-MOF offers an opportunity to identify a potential sensing material. Moreover, it would play an important role in purifying water or wastewater in general.

Oral 11: Cellulose composite films as flexible electronics and adsorbent materials

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Keywords: Cellulose, MOF, Optoelectronic, adsorption

We report on the fabrication of conductive, transparent and flexible films made from bacterial cellulose microfibers, a polymer and silver nanoparticles as replacements to commercial indium-tin oxide (ITO) and fluorine-doped tin oxide (FTO) transparent conductors. The optical and mechanical properties of the films were tuneable by varying the cellulose to polymer ratio. The cellulose films were coated with silver nanoparticles to make them conductive. The cellulose films showed transmittance between 81% and 71% (Figure 1) and an average resistivity of 9.462 ± 0.588 Ω/sq. These properties compared well to that of commercial ITO and FTO glass substrates [1].

Cellulose composite films fabricated through a solvothemal method were also developed as hydrolytically stable supports for MOFs in water remediation. The films were evaluated for the adsorptive removal of methylene blue (MB) from aqueous solution. Adsorption was characterized by adsorption during the first hour with equilibrium achieved within 4 to 5 hours into the adsorption process. The maximum dye removal efficiency was determined to be 77 % (Figure 2). The adsorption behaviour of the film using MB as a model dye will be discussed.

These studies have demonstrated a cost benefit and a sustainability factor to using green and renewable sources.

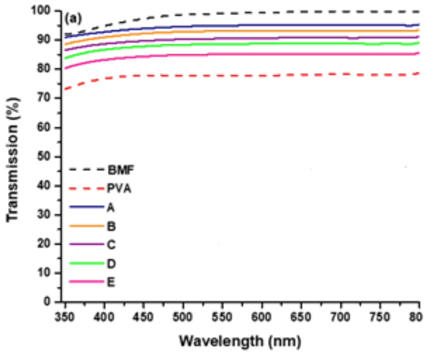

Figure 1: Transmission spectra of cellulose films.

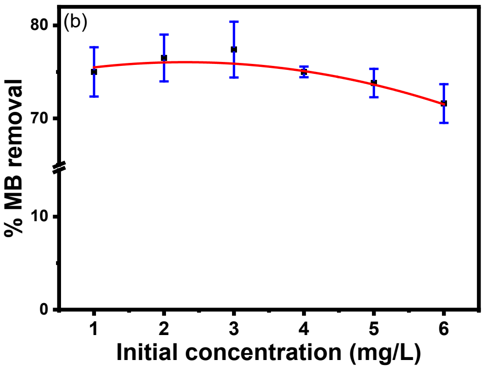

Figure 2: Percentage MB removal vs initial concentration.

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Student 1: Using computational drug design for the synthesis of NHC metallodrugs as potential anticancer and antimicrobial agents

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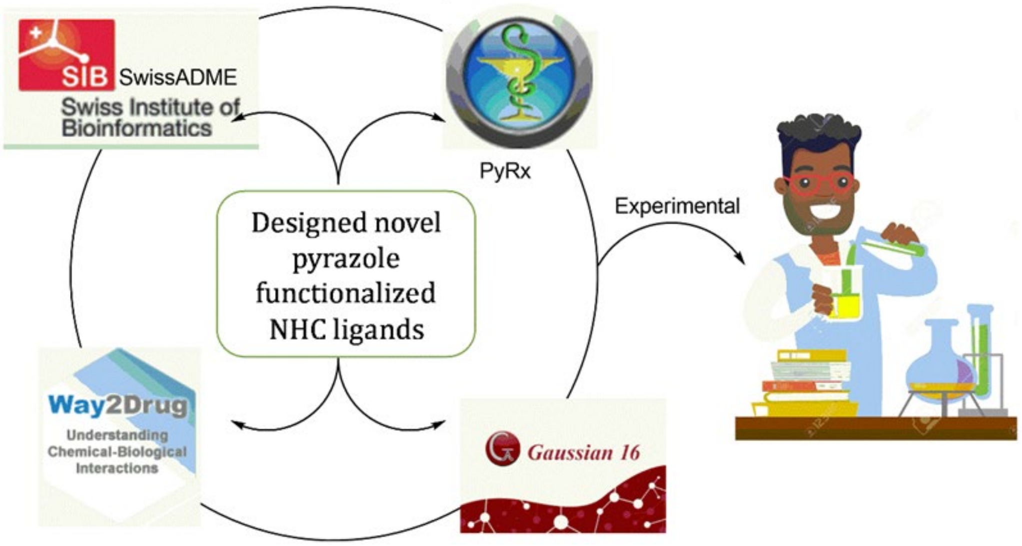
Keywords: NHCs, pharmacokinetic, metallodrugs, DFT

While human health constantly faces challenges due to life-threatening diseases such as cancer and bacterial infections ordinary drug discovery on the other hand takes an average of 12 years from start to commercialisation, raking in an average cost of US$1.8 billion [1]. Theoretical and computational studies are used to shorten the time and reduce the costs associated with drug development [2]. DFT studies have been carried out on the synthesized NHC carbenes and their metal complexes. The molecular descriptors such as (HOMO-LUMO energy gap, ionization energy, electron affinity, electronegativity, etc.) that were obtained from DFT studies showed both the salts and their complexes to be capable of exhibiting some biological activity. Molecular docking against selected protein targets showed the ligand precursors to be bioactive. The so-far synthesized ligands and their complexes have been successfully characterized using NMR, FTIR, HRMS, and they have shown their successful synthesis. *In vitro* antibacterial studies for the imidazolium salts have shown some activity. Future work involves the *in vitro* anticancer analysis of the NHC ligand precursors and their complexes and the invitro antibacterial studies of the complexes. The *in vitro* results will be compared with the theoretical and computational ones.



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Student 2: Quantum chemical studies on antiviral drugs – an insight into antimicrobial resistance

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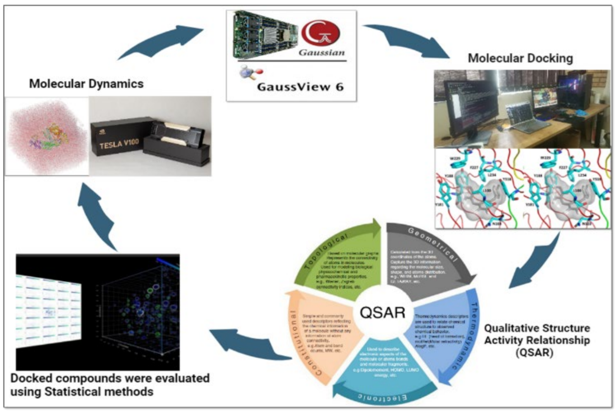
Keywords: Antimicrobial resistance, NNRTIs, Computational chemistry, Quantum mechanics

The escalating incidence of HIV-1 drug resistance poses a significant challenge to the efficacy of combination antiretroviral therapy (ART) initiatives, particularly in southern Africa and beyond. Specifically, the emergence of resistance to non-nucleoside reverse-transcriptase inhibitors (NNRTI) imperils the enduring effectiveness of ART [1]. Antimicrobial resistance (AMR) was directly responsible for an estimated 1.27 million deaths in 2019 [2]. To address (NNRTIs) drug resistance, this study focused on applying computational chemistry techniques such as quantum mechanics, molecular docking, molecular dynamics, and qualitative structure-activity relationship (QSAR) [3,4]. A set of 94 dihydrofuro[3,4-*d*] pyrimidine derivatives were used to develop a (QSAR) model. The results from the four prepared compound classes resulted in the highest R^2 of 0.822 and Q^2 of 0.815 which was achieved for compound class 1. Ligand designer was used to create new compounds for which activity values were predicted using our QSAR model. Enumerated Etravirine showed an activity of 7.373 and a docking score of -10.517 kcal/mol, which was better than its known NNRTI counterpart. Molecular dynamics simulations were conducted to determine the stability of various ligands and their newly developed alternatives, by ensuring that they remain bound to the active site of the protein during a 200ns simulation timeframe. Etravirine produced RMSD fluctuations of approximately 4.5 Å, while the enumerated Etravirine gave RMSD fluctuations of 3.5 Å. Both the lower RMSD and enhanced amino acid interactions suggest that enumerated Etravirine can possibly be used as an alternative for HIV/AIDS treatment.



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Student 3: Photodegradation of tetracycline by a bismuth oxyiodide/red phosphorus photocatalyst

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Keywords: photocatalysis, semiconductors, environmental remediation

The increase in pollution of the aquatic environment is a worldwide environmental concern. This can be attributed to the widespread use of compounds such as pesticides, personal care products, and pharmaceuticals. These compounds are released from household waste, run-off from farmlands, and industrial and hospital effluents and may end up in wastewater treatment plants. Some of the remedial techniques used in wastewater treatment plants to clean complex aqueous matrices of different pollutants cannot remove some of these pollutants sufficiently. Therefore, these contaminants find their way into water bodies and build up in the environment. Research has shown that exposure to these contaminants over time has adverse effects on humans and aquatic organisms. Tetracycline is one of the most commonly used antibiotics to treat infections in both humans and animals because of its effectiveness and broad-spectrum activity. However, some studies have shown that it has been detected in the environment, posing a threat since it does not easily degrade by itself and can bioaccumulate in aquatic organisms.[1] There is a need to find effective ways to remove it from the environment. Environmental remediation technologies are constantly being developed to address water pollution, including the persistent tetracycline pollutant problem. One such promising technique is photocatalysis, a green technology that utilizes sunlight, an abundant energy source. Solar energy is a renewable resource; it is clean and efficient, and most importantly, the products generated after photocatalysis are less harmful. This study aimed at developing novel bismuth oxyiodide-red phosphorus composites. The optoelectronic properties of the materials were studied using different techniques. The composites were then used to degrade tetracycline, a broad-spectrum antibiotic categorized as an emerging contaminant. The best photocatalyst degraded approximately 87% of tetracycline in two hours. Therefore, bismuth oxyiodide-red phosphorus composites are promising photocatalysts for the remediation of polluted water bodies.

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Student 4: Green approach for the synthesis of ZnO-Ag using β-cyclodextrin and honey for photo-catalytic degradation of bromophenol blue

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Keywords: Green chemistry, Ag-ZnO, simultaneous photodegradation, cyclodextrin, honey, green synthesis

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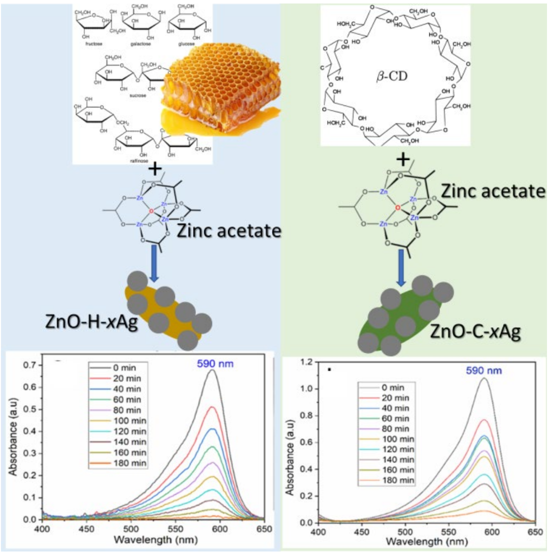
Physicochemical properties are key to the photoactivity of nanophotocatalysts in water decontamination. Green synthetic approaches towards the control of these properties reduces the environmental footprint of nanophotocatalysts.

In pursuit of green synthetic technologies, this work proposes a comparative approach in the use of β-cyclodextrin and honey for the morphological control of ZnO nanoparticles (NPs). It is demonstrated that these naturally occurring materials, β-cyclodextrin and honey, act as surfactants during the synthesis of ZnO as shown by their ability to control the size, shape, and dispersion (denoted ZnO-C and ZnO-H). Coupling of ZnO with Ag NPs through a photo driven wet impregnation technique to form binary nanostructures (ZnO-xAg, ZnO-C-xAg and ZnO-H-xAg) assists in enhancing the physicochemical properties. The photocatalyst varied from spherical, hexagonal, and rod-shaped with the highest surface area of 10 $m^2\ g^{-1}$. Crystalline sizes were 9.38 to 47.95 nm as revealed by XRD. The incorporation of Ag nanoparticles enhanced the life span of photogenerated electron-hole pair by acting as electron trapper. Photodegradation of bromophenol blue (BPB) indicated an enhanced photoactivity of ZnO upon modification with CD, honey, and Ag nanoparticles. The removal of BPB was 98.4% using ZnO-H-3Ag with pseudo reaction rates of up to $518.8 \times 10^{-2} min^{-1}$. It is further demonstrated that the variation in morphology results in pseudo zero, first and second order for the nanophotocatalysts. Total organic carbon (TOC) studies indicated up to 75 % removal of organic carbon by ZnO-H-3Ag at a reaction rate of $8.19 \times 10^{-3}\ min^{-1}$.



Student 5: Adsorption of pharmaceuticals from municipal wastewater effluent by cost-effective magnetite-pine bark biosorbent in a pilot-scale column

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Keywords: adsorption, pilot-scale, fixed bed column, biosorbent, pharmaceuticals, wastewater treatment, biotoxicity

Municipal wastewater treatment plants face challenges in the efficient removal of various pharmaceuticals due to their lower biodegradability [1]. Therefore, there is a need to develop cost-effective and environmentally friendly methods to prevent the discharge of pharmaceuticals into the environment [2]. Utilization of bio-based sorbents is a viable strategy due to the wide availability of various types of renewable and low-cost biomass resources [3]. Pine bark is an abundantly available wood-based by-product that can be chemically modified [4]. It was observed in the previous study that magnetite-pine bark (MPB) which was prepared by modification of pine bark with a mixture of iron salts (Fe^{3+}: $Fe^{2+} = 2:1$), showed high removal efficiency of a variety of pharmaceuticals from wastewater effluent [5]. In the present study, a pilot-scale column with MPB and a mixture of biochar (BC) for providing a better flow of wastewater in the column was used for the adsorption of a variety of pharmaceuticals from secondary wastewater effluent after membrane bioreactor (MBR) of municipal wastewater treatment plant in Oulu, Finland. The regeneration of biosorbents was conducted with 0.2 M NaOH two months after the beginning of the study. Pilot-scale adsorption testing was performed for 4 months with the enumeration of viable bacteria and biotoxicity testing using *N. europaea* strain. The result of the pharmaceutical analyses showed that the BC+MPB bed was efficient in the removal of different pharmaceuticals as well as antibiotics to low concentrations or below the detection limit all over the pilot-scale study. Batch adsorption experiments with BC and MPB were conducted separately with the wastewater effluent to compare the efficiency of each sorbent. The results proved that MPB was efficient in the batch adsorption of pharmaceuticals, however, BC was not effective. For example, the removal efficiency of trimethoprim was 82.2 and 12.2% over MPB and BC, respectively. Before the regeneration, the wastewater had higher CFU/mL compared to pilot samples. After the regeneration, the CFU/mL of pilot samples was higher than the wastewater with a drastic increase immediately after regeneration. Biotoxicity testing revealed that the wastewater was not toxic to *N. europaea* since it had undergone membrane treatment and adsorption did not introduce any new toxicity except after the regeneration. The percentage inhibition went up and down a little during the entire study, but the variations were insignificant. The highest percentage of inhibition was observed after the regeneration at about 73.7% and then it was stabilized at about 15% after 10 days. The result was probably due to the release of adsorbed contaminants from the surface of the biosorbent after regeneration.

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Student 6: Synthesis of substituted triazines and their investigation as corrosion inhibitors on Al in 1M HCl: Experimental and DFT studies

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Keywords: Synthesis, kinetics and thermodynamics, electrochemical analysis, binding energies.

The substituted triazines, namely 4,6-dichloro-1,3,5-triazin-2-yl)morpholine (DMT), 4.6-dichloro-N-phenyl-1,3,5-triazin-2-amine (DPT), and 4,6-dichloro-N-methyl-N-phenyl-1,3,5-triazin-2-amine (DNT) was synthesised and studied as a corrosion inhibitor on Aluminium(Al) corrosion in 1M hydrochloric acid (HCl) solution. The anticorrosive effect was investigated using weight loss analysis, electrochemical impedance spectroscopy (EIS), potentiodynamic polarization curve (PDP), and density functional theory approach (DFT). The current investigation has demonstrated that the percentage inhibition efficiency(%IE) for the tested inhibitors were found to be inhibitor concentration dependence, and the maximum %IE for DMT, DPT, and DNT was 83.02% at 303K,82.39% at 303K, 95.02% at 313K respectively. When DMT and DPT were present, the effect of temperature shows that the inhibition efficiency decreased as the temperature increases. As opposed to this, the inhibition efficiency was unstable in the presence of DNT since it increases when the temperature went from 303K to 313K and fell when it reached 323K. the EIS measurement showed that comparing the corrosive solution with the inhibitor versus the uninhibited corrosion solution, the electrolyte resistance increases. Inhibition efficiency increases when polarisation resistance rises in response to an increase in inhibitor concentration for each inhibitor. PDP measurement showed that all inhibitors are either anodic or cathodic inhibitors. Langmuir's isothermal adsorption was followed by the tested corrosion inhibitors as they adsorbed on the Al surface in a HCl solution. DFT techniques was used to perform inhibitor---Al interactions to estimate the binding energies of the inhibitors on the Al(111) surface.

Student 7: Schiff-base pyrazole chelator ligands coordinated to the *fac*-$[Re(CO)_3]^+$ synthon: synthesis, crystallography and *in vitro* studies

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Keywords: Schiff-base, coordination, rhenium, radiopharmaceuticals

There have been a lot of research reported on the coordination of Schiff-base compounds on the rhenium metal ion, where the metal is highly electropositive [1-3]. Rhenium is a prospective contender for radiochemistry because of the ideal nuclear properties (high-energy beta particles) rendered by the two radioisotopes of this metal, $^{186/188}$Re [4]. Investigating the basic coordination chemistry of rhenium is significant for discovering new target-specific rhenium radiopharmaceuticals as the biodistribution of a radiopharmaceutical is highly dependent on its stability, charge, molecular weight, geometry as well as the nature of the co-ligands occupying the coordination sphere [4]. A series of Schiff-base pyrazole chelator ligands were synthesized, screened against numerous cancer cell lines and then coordidinated to the *fac*-$[Re(CO)_3]^+$ synthon with the aim of investigating the stability and pharmacological activity of the metal complexes against the same cancer cell lines as that used for the testing of the ligands. **Figure 1**. illustrates the molecular crystal structures of (a) monometallic and (b) bimetallic rhenium(I) tricarbonyl complexes synthesized in this study. In (b) the two pyrazole ligands serve as bridging ligands between the the two adjacent rhenium metal ions.

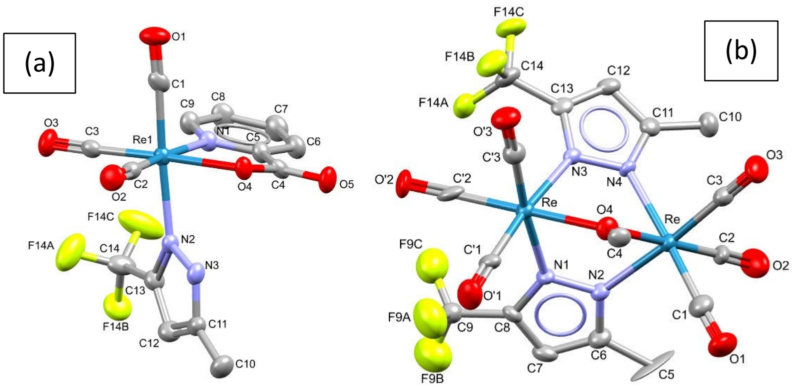

Figure 1: Molecular structures of (a) *fac*-$[Re(CO)_3(Pico)(L4)]$ and (b) *fac*-$[Re(CO)_6(CH_3OH)(L4)_2][Et_4N]$. L4 = *3,5-bis(trifluoromethyl)-1H-pyrazole*.

The ability of these pyrazole ligands to chelate with both nitrogen atoms, where one nitrogen atom coordinates *via* dative covalent bonding to form bimetallic complexes is the highlight of this study. The chelator ligands used in this study are picolinic acid, *3,5-bis(trifluoromethyl)-1H-pyrazole*, and *3,5-dimethyl-1H-pyrazole*, however for the sake of this abstract only two crystal structures of the same monodentate ligand are presented.

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Student 8: Selective electrochemical detection of ciprofloxacin with functionalised reduced graphene oxide/strontium oxide-palladium nanocomposites

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Keywords: sensor, nanocomposite, chemical synthesis

The detection and quantification of antibiotics in environmental and biological matrices have gained significant attention due to their potential adverse effects on human health and the environment.[1] Therefore, a quick and in situ detection method is of great importance. In environmental media, several detection techniques, such as mass spectrometry, solid phase extraction, and chromatography (HPLC/GC), have been used for detection. However, electrochemical methods have shown to be an encouraging technique because of their sensitivity, rapidity, and compactness. In this study, a various percentage (10% - 40%) of reduced graphene oxide (rGO), incorporated with strontium oxide (SrO) and palladium (Pd) nanoparticles, were synthesised via the wet chemical method and modified on a glassy carbon electrode (GCE). The nanocomposites were characterised using various spectroscopic and microscopic techniques. The electrochemical performance of the 40% rGO-SrO-Pd/GCE towards ampicillin detection was evaluated using cyclic voltammetry (CV) and differential pulse voltammetry (DPV). The modified electrode exhibited enhanced electrocatalytic activity towards ampicillin oxidation compared to the bare GCE, attributed to the synergistic effects of rGO, SrO, and Pd nanoparticles. The calibration plot showed a linear relationship between the peak current and ampicillin concentration in the range of 0.05 - 21.7 μM, with the limit of detection and quantification of 17 nM and 50 nM, respectively. The proposed sensor demonstrated excellent selectivity, stability, and reproducibility in real water and urine samples for ampicillin detection. Overall, the 40% rGO-SrO-Pd/GCE presents a promising platform for the sensitive and selective detection of ampicillin in environmental and biological samples, offering potential insights into antibiotic monitoring and environmental protection efforts.

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P1: Development of novel ruthenium-based metallodrugs for application in photodynamic therapy

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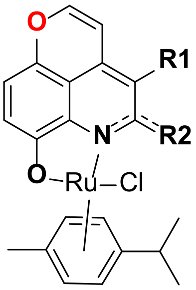
Keywords: cancer, chemotherapy, PDT, Ruthenium, quinoline

Cancer is a global burden, with an estimated 27.5 million new cases and an accompanying 16.3 million deaths by 2040, according to the International Agency for Research on Cancer (IARC) [1]. Although there are several therapeutic options available to treat cancer, the variety of cancers, targeted organs or tissues, and metastases thereof renders the treatment of the disease challenging. Surgery, radiotherapy, and chemotherapy are widely used with reasonable success, but they come with limitations such as drug resistance, selectivity to cancer cells, toxicity to normal cells, drug solubility in vivo, mode of administration, metastases, and cancer cell recurrence [2], [3]. As such, novel approaches, strategies, or personalized treatments are required to overcome limitations in cancer treatment.

Metal complexes can accumulate in specific organelles within cells and induce cytotoxicity in the presence of light. Such a mode of action is further enhanced for molecules rich in extended π-systems. The presence of extended π-systems escalates fluorescence emission and enables the exact location of a molecule within the cell. These properties, viz., cellular accumulation, phototoxicity, and fluorescence emission, allow specific targeting and selective killing of cancer cells over normal cells through photodynamic therapy (PDT) by careful control of light of a specific wavelength over an affected area containing the accumulated drug [4].

The synthesis, photophysical properties as well as biological activity of quinoline-based ruthenium complexes with extended π-systems will be described as potential PDT agents.



R1 = CONHAr, COOMe, or COOH
R2 = Cl or O

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P2: Synthesis and study of thiolato-gold(I) complexes as anticancer agents

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Keywords: gold(I), synthesis, anticancer, *in vitro*

Cancer, a disease that occurs as a result of rapid and abnormal cell growth, is one of the leading causes of global mortality [1]. Current treatment for cancer includes chemotherapy, which often involves platinum-based drugs such as cisplatin or carboplatin. This course of treatment often results in adverse side effects due to drug toxicity. An increase in resistance to these platinum-based drugs has also been reported in recent years [2]. As a result, research involving new chemotherapeutic agents that are less toxic and effective against resistant cells is required. Gold is a metal that has been used in medicine for many years. Most notably the gold(I) drug Auranofin which has been used as a primary treatment of Rheumatoid Arthritis since 1985 [3,4]. Studies suggest that gold-based drugs may potentially target cancer cells through the enzyme thioredoxin reductase, which is known to be over-expressed in cancer cells associated with cisplatin resistance [3]. This presentation discusses the synthesis and study of thiolato-gold(I) complexes that include a phosphorus-gold-sulphur moiety (figure 1). Along with synthesis and characterization, the complexes chemical stability and *in vitro* activity against cancer cells will also be discussed.

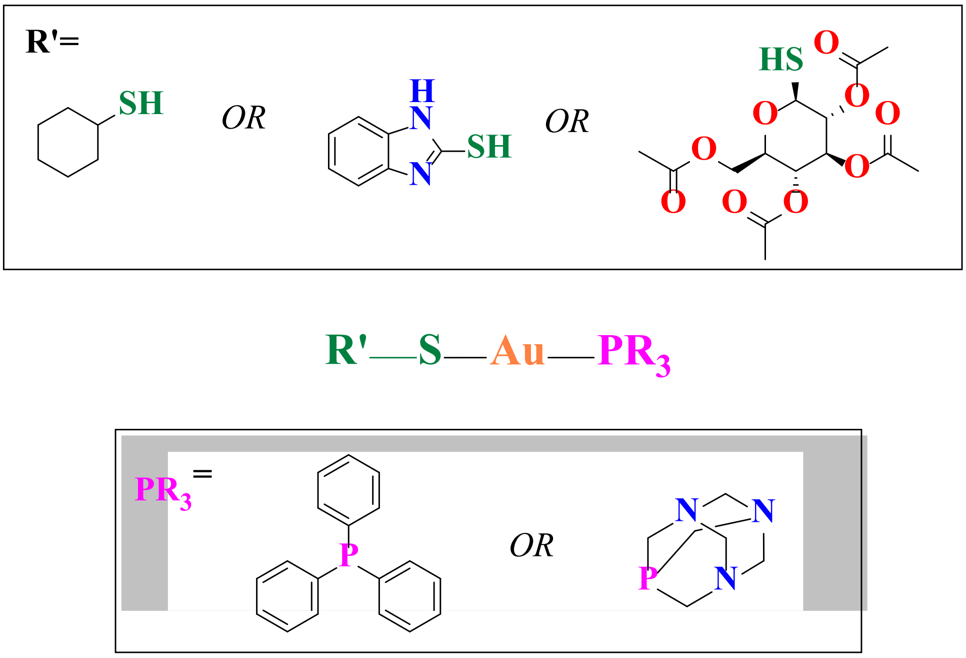

Figure 1 A summary of the thiolato-gold(I) complexes that will be discussed.

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P3: Spectroscopic and computational pH study of Ni(II) and Pd(II) Pyrrole-imine chelates with human serum albumin

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Keywords: albumin, ligand binding, DFT simulations, Schiff base chelate, circular dichroism, fluorescence

Pyrrole-based compounds have garnered substantial attention in scientific research due to their inherent bioactivity and prominent role in pharmaceutical applications. It has also been shown that pyrrole-imine Schiff bases can chelate a wide range of transition metal ions and exhibit significant medicinal potential. However, there remains a limited body of work focused on elucidating the binding mechanisms of these compounds to human serum albumin (HSA). HSA is the most abundant protein in human plasma and efficiently transports drugs *in vivo*. It is, therefore, essential to delineate the binding of metallodrugs to HSA.

In this study, a tetradentate bis(pyrrole-imine) ligand, H_2PrPyrr, was synthesised along with its isoelectronic (nd^8) square-planar chelates of Ni^{II} and Pd^{II}, denoted as M(PrPyrr) (**Figure 1**). The binding interactions of H_2PrPyrr and M(PrPyrr) with HSA across various pH values were determined spectroscopically in order to assess the influence of the metal ion on the uptake of the respective metal complex and to ascertain their preferred binding site(s).[1]

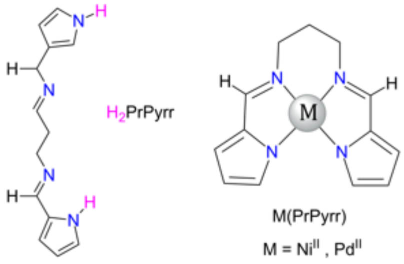

Figure 1: Structures of the bis(pyrrole-imine) ligand H_2PrPyrr (N,N'-bis[(1E)-1H-pyrrol-2-ylmethylene]propane-1,3-diamine) (left) and its neutral Ni^{II} and Pd^{II} chelates (right).

Results suggest that HSA binding depends not only on the identity of the d^8 metal ion, but on the pH level as well. The affinity constants, K_a, ranged from ~3.5×10^3 M^{-1} to ~1×10^6 M^{-1} at 37 °C, following the order Pd(PrPyrr) > Ni(PrPyrr) at pH levels of 4 and 7; but Ni(PrPyrr) > Pd(PrPyrr) at a pH level of 9. Fluorescence quenching data for probe-bound HSA showed that sites close to Trp-214 (subdomain IIA) were targeted. Ligand uptake was found to be enthalpically driven, dependent mainly on Londons dispersion forces. The induced CD spectra for the protein-bound ligands were simulated using hybrid QM:MM TD-DFT methods to corroborate spectroscopic data and to confirm that the metal chelates neither decomposed nor demetallated upon binding to HSA. The transport and delivery of the metal chelates by HSA in vivo is, therefore, feasible.

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P4: Anticancer activities of Re(I) tricarbonyl complexes with *N,O*-bidentate ligands: synthesis, *in vitro* and *in silico* biological evaluation

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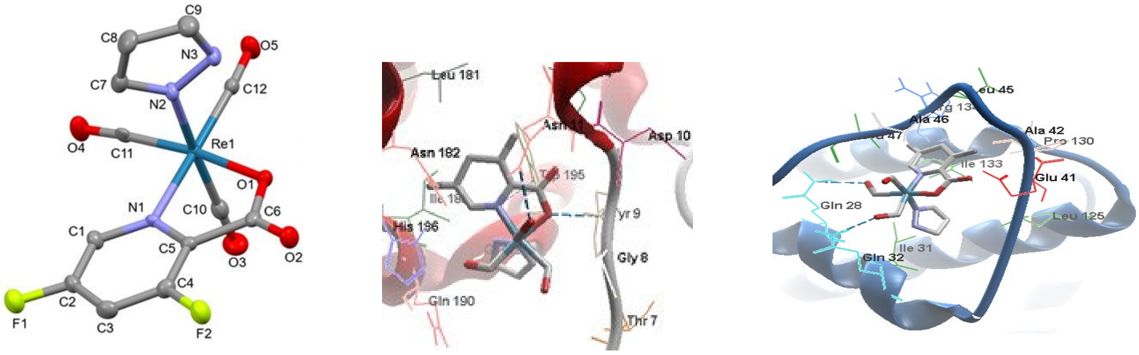
Keywords: Rhenium(I), *N,O*-bidentate, crystallography, *in vitro*, *in silico*

Recently, several investigations on rhenium tricarbonyl complexes have been carried out to develop new anticancer drugs due to their advantageous properties [1]. Therefore, this work investigated the distinct characteristics of metal-based rhenium tricarbonyl complexes carrying different *N,O* bidentate ligands with fluorinated derivatives as potent anticancer drugs using *in vitro* investigations and *in silico* molecular docking techniques. The '2+1' mixed ligand approach was used to synthesize *N,O*-coordinated *fac*-$[Re(CO)_3]^+$ complexes. 3,5-Difluoro-2-picolinic acid (Dfpc) and pyrazole (Pz) were added to the aqua metal complex to yield a crystal complex depicted in **Figure 1a:** *fac*-$[Re(Dfpc)(CO)_3(Pz)]$.



1a **1b** **1c**

Figure 1: Solid state depiction of *fac*-$[Re(Dfpc)(CO)_3(Pz)]$ (**1a**), with pro-apoptotic BAX-1 protein (**1b**), and anti-apoptotic human BCL-2 protein (**1c**).

Fifteen picolinic acid-based complexes were synthesized, and the single-crystal X-ray diffraction studies were conducted for eight of the complexes. The results showed that the structures have typically small bite angles ranging between 74.61° and 75.90° with a slightly distorted octahedral geometry. The π-accepting character of the *N,O* ligand is enhanced by the presence of fluorine(s) on its backbone, as demonstrated by the reduction in the Re1-O1 bond lengths (ranging between 2.108 Å and 2.146Å) with each additional fluorine [2]. The molecular docking analysis revealed that the complexes had a strong binding affinity (−3.25 to −10.16 kcal/mol) and had the potential to seriously impair the proteins under investigation's typical physiological functions. Out of the fifteen synthesized picolinic acid-based complexes, only one complex bearing picolinic acid and aqua ligands displayed favorable cytotoxicity towards HeLa and A549 cancer cells [3].

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P5: Synthesis, characterization, DFT, molecular docking and antimalarial studies of novel salen-based ruthenium complexes

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Keywords: Salen, Ruthenium, Malaria

The reported shortcomings of platinum-based drugs (mainly cisplatin) have been a driving force towards the development of alternative metallodrugs. Research has shown group 8 transition metal complexes exhibit interesting anticancer and antimalarial activities. Iron complexes, such as ferroquine are undergoing clinical trials against chloroquine resistant malaria strains whereas ruthenium complexes such as NAMI-A and KP1019 are undergoing clinical trials as anticancer agents.[1]

In this work a series of novel salen based ligands and their ruthenium complexes (Fig. 1) have been synthesized and characterized using a range of spectroscopic techniques including single crystal X-ray crystallography. DFT studies, molecular docking studies and antimalarial bioassays for both ligands and their complexes have been conducted, in order to understand their possible activity against chloroquine resistant malaria strains. Our findings predict enhanced bioactivity with the metal coordinated salen ligands as compared to free ligands.

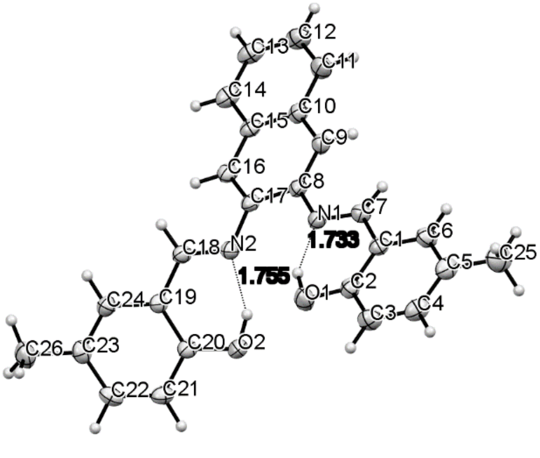

Figure 1: Salophen ligand

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P6: The multi-stage antiplasmodial activity and mechanistic investigation of ferrocenyl quinoline-benzimidazole molecular hybrids

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Keywords: malaria, molecular hybridization, ferrocene, multi-stage activity

Malaria, a mosquito-borne disease, is one of the most devastating infectious diseases, with an estimated 249 million cases and 608 000 related deaths reported globally in 2022 alone [1]. The World Health Organization estimated that the African region accounted for 93.6% of these cases and 95.4% of the global deaths [1]. Despite the rollout of the RTS,S/AS01 malaria vaccine (2019) and the recent introduction of the R21/Matrix-M vaccine, there is still an urgent need to develop antimalarials for the effective treatment of malaria. Caused by a protozoan parasite of the genus *Plasmodium*, *Plasmodium falciparum* is the most virulent strain, and responsible for the greatest number of deaths globally. Despite the various treatment regimens available, the increasing threat of drug resistance, both intrinsic and acquired, has prompted investigations into alternative approaches toward antimalarial drug design.

In an attempt to circumvent this rising resistance, the molecular hybridization of biologically important pharmacophores, such as the quinoline and benzimidazole scaffolds, has proven to be a fruitful avenue within antiplasmodial drug discovery [2]. Quinoline-based antimalarials, in particular, have been demonstrated to be a vital part of the chemotherapeutic armoury against this disease. Additionally, metal incorporation, which has been extensively explored for the purposes of overcoming resistance mechanisms within the parasite, is exemplified by the antimalarial drug candidate, Ferroquine (FQ) [3]. FQ has demonstrated remarkable activity, notably against resistant forms of the *Plasmodium* parasite. The incorporation of the ferrocenyl moiety was shown to impose an additional mechanism of action and thus its potency is attributed to its dual action mechanism [3]. Furthermore, FQ has reached phase 2a clinical trials, with the most recently reported trial involving the administration of FQ to patients as part of a co-administration study [4].

It is imperative to develop antimalarials that can act across multiple stages of the parasites' life-cycle. In the current climate, tackling the transmission of this parasitic disease is a crucial strategy within drug development, as most antimalarials, despite displaying potent activity against the asexual blood stage, do not affect the transmissible gametocyte stages. The ideal antimalarial should kill the parasite at both the intraerythrocytic asexual blood and transmissible gametocyte stages, as this will not only treat the infected patient but also provide protection for the population by preventing further transmission.

This presentation will focus on the design of a series of bioorganometallic ferrocenyl aminoquinoline-benzimidazole molecular hybrids, highlighting the avenues of both molecular hybridization and metal incorporation [5]. Therewith, their antiplasmodial activity against the *in vitro* asexual blood and sexual gametocyte stages, as well as putative mechanistic studies, such as β-haematin inhibition and cellular haem fractionation, will be discussed.

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P7: Fine-tuning the chemical and physical properties of zeolitic catalysts for the ethanol dehydration process to form ethylene

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Keywords: Biomass, Bioethanol, Dehydration, Ethylene, Acid Catalysts

Ethylene is a paramount feedstock for the manufacturing of lubricants, surfactants, plasticizers, and polymers such as polyethylene [1]. Traditionally, ethylene is produced from thermal steam cracking of non-renewable based fossil fuels [2]. Fossil fuels offer a high throughput, but they also cause a massive damage to the environment which emanate from the high emissions of toxins released during their combustion. On the other hand, in compliance with the sustainability goals, agricultural renewable materials can be used as an alternative feedstock to produce biofuels, bio-oils, and biogases [3]. For example, bioethanol which is easily obtained from the fermentation of edible and non-edible biomass is a clean and environmentally benign, renewable biofuel. Bioethanol as the green fuel source undergoes various processes such as catalytic dehydration, dehydrogenation, oxidation, reforming, coupling, decomposition, gasification etc. to produce value-added products such as diethyl ether, ethylene, propylene, ethyl acetate, ethylene oxide, acetone, and acetaldehydes etc. which are used for industrial and domestic purposes.

ZSM-5 is a promising and a versatile heterogeneous catalyst for bioethanol dehydration since it is porous and constitutes both Lewis and BrØnsted acidic sites [4]. Notably, the porosity and acidity of the zeolitic catalyst plays a significant role in ethanol conversion to ethylene. However, the presence of strong acid sites in the zeolite catalysts poses a major challenge in their stability and in the deposition of coke [5]. As a result, a lot of research interest has been invested in the pursuit of circumventing the challenges associated with the used of bare zeolite catalysts for ethanol dehydration process. Therefore, the various transition and rare earth metals from the periodic table are added to reduce the acidity of the zeolite catalysts thereby improving the catalytic properties of an acid catalyst. Zeolites accommodate both monovalent and bivalent metal modifications.

This research project was based on the use of commercial ZSM-5 modified with late transition metals to produce ethylene through the process of ethanol dehydration. The metals that were loaded on the ZSM-5 catalyst are nickel and iron in both monometallic and bimetallic forms. This is because iron is known to favour the formation of ethylene during ethanol dehydration whilst nickel gives the best ethanol dehydration and ethylene yield. The solid acid catalysts greatly improved the production of ethylene at lower temperatures using modified ZSM-5.

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P8: Development of N,O-donor earth abundant metal catalysts for the synthesis and depolymerization of poly(lactides)

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Recently, significant amount of research has been devoted to the production of biodegradable and biocompatible polymers derived from renewable sources as alternatives to the well-established petroleum-based polymers. This is driven by the need to reduce the accumulation of (micro)plastic wastes in the environmental alongside promoting a circular economy. Polylactides (PLA) have emerged as suitable candidates as the monomers are derived from renewable resources such as corn in addition to being biodegradable. Herein, we report the syntheses of Mn(II), Mn(III) and Zn(II) complexes bearing imino/amino pyridine/phenolate Schiff base ligands. Structural characterization of the complexes using NMR and IR spectroscopies, elemental analyses and single crystal X-ray crystallography revealed the formation of mononuclear and multinuclear complexes with diverse coordination modes. The complexes showed high catalytic activities in the ring-opening opening polymerization of *rac*-lactide to produce mainly atactic PLA. Significantly, the Mn(III) and Zn(II) complexes catalysed the degradation of PLA to give predominantly methyl lactate (**Fig. 1**). The catalytic performance of the complexes was regulated by the identity of the donor ligand, metal atom and coordination chemistry.

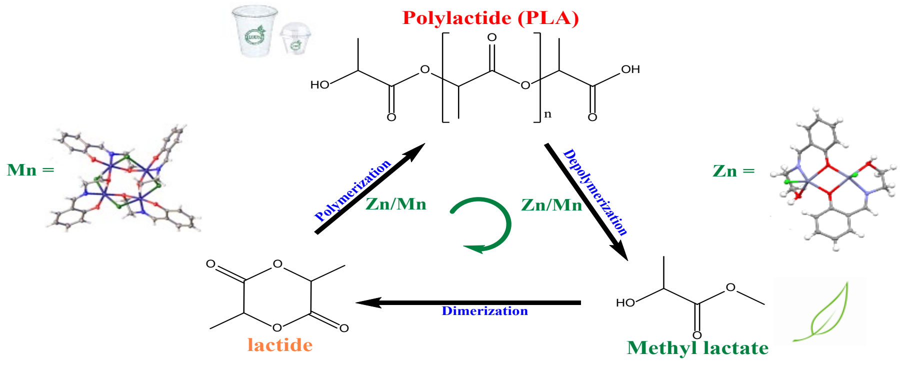

Fig. 1: Mn(II), Mn(III) and Zn(II) catalyzed production and and depolymerization of poly(lactides).

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P9: Re^I tricarbonyl modalities with newly designed and synthesized *N,N'*-pyrazole ligand frameworks as potential anticancer drugs

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Keywords: Pyrazole, Rhenium, Tricarbonyl Chemistry.

More than 100,000 people worldwide receive a cancer diagnosis annually, with an estimated 19.3 million new cases and nearly 10.0 million cancer-related deaths, resulting in a survival rate of approximately 60% [1]. These staggering statistics underscore the critical importance of increasing the rate of new radiopharmaceutical approvals for commercial use. The development of potential new radiopharmaceutical drugs will not only advance our understanding but also guide the selection of optimal chemo-therapeutic and diagnostic agents in the fight against cancer. [2].

In recent years, there has been extensive exploration into rhenium(I) tricarbonyl chemistry, with its compounds emerging as promising candidates for antibacterial and anticancer therapies. Molecular interactions between DNA and Re^I tricarbonyl complexes are particularly crucial in various significant investigations, including cancer treatment [3]. Additionally, numerous pyrazole compounds are renowned for their remarkable medical and photophysical applications, exhibiting potential anti-cancer, anti-bacterial, anti-parasitic, and anti-viral (HIV-1) activities [4].

In this project, our objective is to design and synthesize a variety of pyrazole ligand derivatives to form bidentate chelating frameworks. These ligands will then be coordinated with rhenium metal ions to create tricarbonyl Re^I organometallic complexes, capitalizing on their exceptional medicinal properties for targeted anti-cancer radiopharmaceutical treatments. All synthesized compounds will undergo thorough analysis using techniques such as IR, UV/Vis, SC-XRD, and NMR.

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P10: Synthesis, characterization, and biological studies of Pt(II) complexes with bidentate iminopyridine ligands

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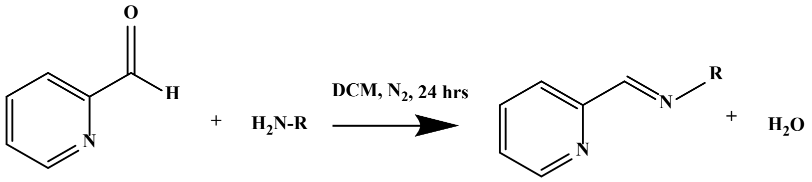
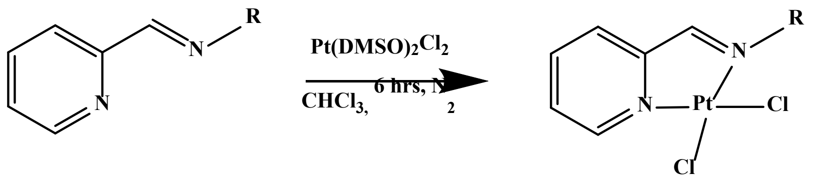
Keywords: Cisplatin, *N,N*-donor ligands, Pt(II) complexes, DNA interactions.

The use of Platinum based drugs in cancer treatment gained significant interest since the discovery of Cisplatin in 1969 by Bernett Rosenberg. Cisplatin is used to treat cancer of the ovaries, testicles, lung, head, neck, just to mention a few. Studies have shown that the bonds formed between Pt(II) complexes and N-donor ligands are thermodynamically stable when they reach the DNA helix where they covalently bind to the structure, resulting in the hinderance of DNA replication, ultimately leading to cancer cell death. Even though Cisplatin is one of the most potent chemotherapy drugs widely used to treat cancer, it has shown several disadvantages, namely: severe side effects such as hearing loss, nausea, nephrotoxicity, allergy, elevated blood pressure, etc. Moreover, this drug has a limited spectrum of tumor types that it can act on, and some cells are resistant to it. These disadvantages indicate a scope for improvement to increase clinical effectiveness by broadening the spectrum of action and reduce toxicity by eliminating side effects. In this study we explore the effect of steric hinderance, electronic properties and stability of N-donor Pt(II) complexes to DNA interaction, substitution kinetics and cytotoxicity. Pyridine ligands **L1** to **L4** were prepared via a condensation reaction of 2-pyridinecarboxaldehyde with various amines and were produced in moderate yields (**Scheme 1**). Equivalent amounts of **L1** to **L4** were reacted with $Pt(DMSO)_2Cl_2$ to give platinum (II) complexes **PtL1** to **PtL4** (**Scheme 2**). The compounds were characterized using NMR, mass spectroscopy, FT-IR, and elemental analysis. **PtL1**, **PtL2** and **PtL3** crystallized in monoclinic, monoclinic, and triclinic crystal systems with $P2_1/n$, P2/n and P-1 space groups, respectively. The coordination geometry around the platinum atom in all three complexes exhibited a distorted square planar geometry.



R = ^{i}Pr (L1)
R = C_6H_5 (L2)
R = 2,6-$Me_2C_6H_3$ (L3)
R = 2,6-$^iPr_2C_6H_3$ (L4)

Scheme 1: Synthesis of (imino)pyridine ligands (**L1-L4**).



R = ^{i}Pr (PtL1)
R = C_6H_5 (PtL2)
R = 2,6-$Me_2C_6H_3$ (PtL3)
R = 2,6-$^iPr_2C_6H_3$ (PtL4)

Scheme 2: Synthesis of platinum complexes (**PtL1 - PtL4**).

P11: Synthesis, spectroscopic characterisation, and CO-release of Mn(I) tricarbonyl complexes, coordinated with biologically active amino-based ligands

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Keywords: Manganese(I) tricarbonyl, cytotoxicity, anticancer agents, synthesis

Over the years, low oxidation state carbonyl complexes of group 7 elements (rhenium (Re), technetium (Tc), and manganese (Mn)) have attracted attention in medicinal chemistry, as a result of high stability of the *fac*-[M(CO)$_3$] core (where, M = Re, Tc, Mn). In radiopharmaceutical applications, Re and Tc have been thoroughly explored because of their diagnosing and therapeutic abilities. Hence, for the past ten years, the cytotoxicity of rhenium-tricarbonyl complexes has been studied as potential anticancer agents to replace platinum-based anticancer agents such as cisplatin, carboplatin, and oxaliplatin due to platinum-based treatment being ineffective against drug-resistant tumours and for producing severe side effects [1]. Literature reveals that manganese (a biocompatible element that plays an important role in biological systems) compared to its Group 7 analogue, Re, has been under-explored, with only a few cytotoxicity studies reported on the manganese-tricarbonyl synthon. Furthermore, recent reported studies have shown the potential of Mn(I) tricarbonyl complexes as anticancer agents. For example, Mn complexes have been reported to display cytotoxic effects towards cancerous cells *via* their CO release mechanism (i.e., reactive oxygen species generation, mitochondria damage, DNA cleavage, autophagy, and apoptosis induction) [2-3]. Therefore, this project aims to synthesise, and structurally evaluate *fac*-[Mn(CO)$_3$(*L,L'*)(NCS)] complexes, (where, *L,L'* = *N*-heteroaromatic derivatives of amino ligands (histidine, alanine, and cysteine) with quinoline-2-carboxaldehyde, and NCS thiocyanate ligands, as illustrated in Figure 1. Characterisation of the synthesised complexes was done using spectroscopic techniques such as Nuclear Magnetic Resonance (NMR), Ultra-Violet Visible (UV/Vis), and Fourier Transform Infrared spectroscopy (FTIR).

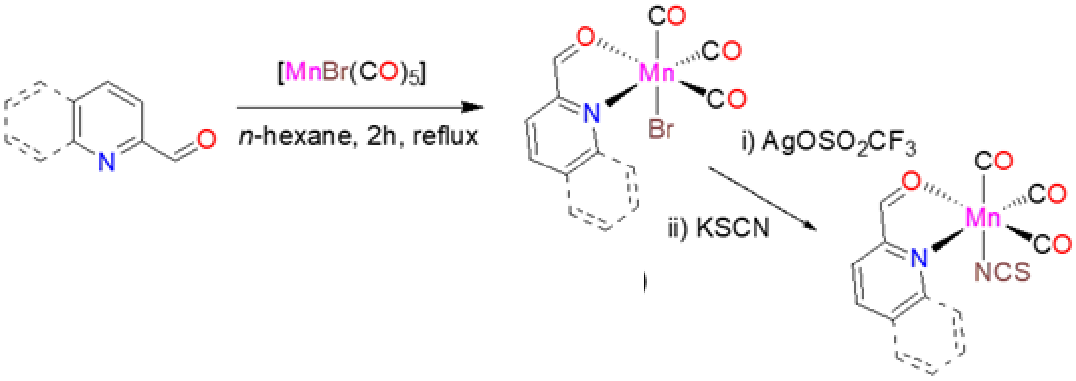

Figure 1: Synthetic route of the synthesised complexes and precusors.

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P12: Completing the picture – The halogenated benzoylanilides

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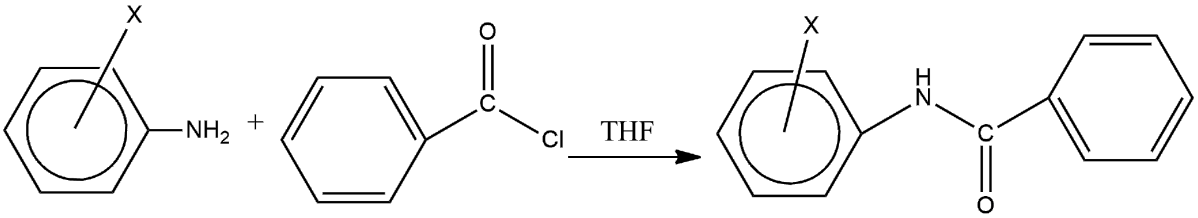
Keywords: anilides, structure elucidation, multinuclear NMR, Hydrogen bonding, synthesis.

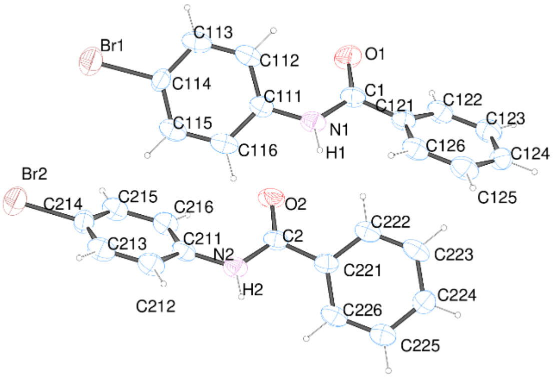
The full series of monohalogenated benzoylanilides has been synthesized from benzoyl chloride and monohalogenated anilines, respectively, according to standard procedures (Scheme 1)[1] and characterized in solution and in the solid state.



Scheme 1: The synthesis procedure of the monohalogenated benzoyl anilides from the respective monohalogenated aniline derivatives, using benzoyl chloride. (X = F, Cl, Br, I)

The crystal and molecular structures of all compounds have been determined by diffraction studies performed on single crystals, inter- and intramolecular bonding patterns have been analyzed and assessed for similarities in the homologous series (Scheme 2). An increment system for the ^{15}N NMR shifts in the anilides relative to the free anilines has been devised experimentally and corroborated by means of DFT methods, thus yielding an equation that allows for predicting pertaining ^{15}N NMR shifts increments to unknown benzoylanilides.

To assess the thermal stability of the title compounds TGA studies were conducted and found to show clear trends with incremental shifts typical for the regioisomer. IR and UV-Vis spectra were recorded to identify typical shift patterns with regards to regioisomers as well as the nature of the halogen.



Scheme 2: The solved crystal structure for p-bromobenzoyl anilide showing the two formula units found in the asymmetric unit cell.

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P13: Optimization of maceration technique for extraction and characterization of Mimosa Wattle (Acacia Mearnsii) tree bark constituents

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Keywords: Optimization, Response Surface Methodology (RSM), Maceration Extraction, Mimosa Wattle, Acacia mearnsii, Characterization, Bioactive Compounds

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Mimosa wattle (*Acacia mearnsii*) tree bark is a promising source of bioactive compounds with various industrial applications. This research aims to optimize the maceration extraction process for the efficient recovery of bioactive constituents from mimosa wattle tree bark using Response Surface Methodology (RSM), followed by characterization of the extracted compounds. RSM was employed to systematically evaluate and optimize key extraction parameters including solvent type, solvent-to-bark ratio, extraction time, and temperature. Design of Experiments (DOE) was utilized to generate a central composite design (CCD) matrix to explore the interactive effects of these parameters on extraction efficiency. The optimized extraction conditions were validated experimentally. Subsequently, the extracted compounds were characterized using advanced analytical techniques including high-performance liquid chromatography (HPLC), gas chromatography-mass spectrometry (GC-MS), Fourier transform infrared (FTIR) spectroscopy, and nuclear magnetic resonance (NMR) spectroscopy. The characterization provided insights into the chemical composition, structural properties, and potential bioactivities of the bioactive constituents present in mimosa wattle tree bark extract.

P14: Green synthesis of silver nanoparticles and the evaluation of their antimicrobial activity

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Keywords: *Ozoroa reticulata*, Silver nanoparticles, Antimicrobial activity

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The increasing demand for silver nanoparticles has led to the need for new superior and environmentally benign methods of synthesis to be developed. In this study, the *Ozoroa reticulata* plant was used in the plant extract-mediated synthesis of silver nanoparticles. The silver nanoparticles were characterized using FTIR, XRD, TGA and SEM-EDX. The phytochemical tests showed that the plant is rich in phytochemicals such as flavonoids, alkaloids, steroids and glycosides which possess great potential for reducing and capping silver nanoparticles. The synthesised silver nanoparticles showed great inhibition against the *Escherichia coli* and the *Staphylococcus aureus* bacteria, exhibiting maximum inhibition zones of 23 mm and 24 mm respectively. *Ozoroa reticulata* showed great potential as an alternative for the synthesis of silver nanoparticles and the plant-mediated silver nanoparticles showed great potential as alternatives to antibiotics.

P15: A computational study of mechanistic pathways for the design of a greener process in the production of quinolin-2-(1H)-one and its derivatives

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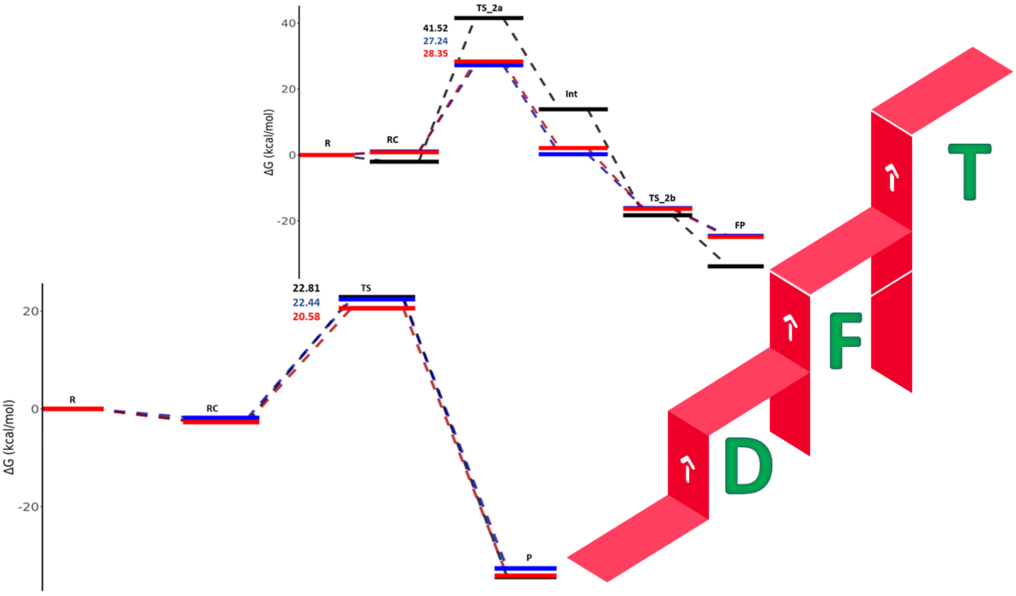
Keywords: quinoline-2(1H)-one, green, methods, computational, mechanistic, pathway, theoretical, investigation

Quinolinones are heterocyclic aromatic compounds with various pharmacological activities. Their importance has brought about the need for green synthetic methods [1]. Exploring greener pathways using an experimental trial and error approach is costly and hazardous hence computational investigations of the existing mechanistic pathways are an alternative [2]. This study focused on the computational study of a fast, base-free aqueous synthesis of quinolin-2(1H)-one. Molecular simulations were done using DFT [3], MP2, and CCSD(T) [4] to obtain reaction energy profiles of quinoline-2(1H)-one in gas, water, and dichloromethane phases. The profiles for the two-step reaction helped to elucidate the energy barriers for the chemical reaction. The barrier for the reaction in water and dichloromethane in the first step was 22.44 and 20.58 kcal/mol, respectively, while for the second step 27.24 and 28.35 kcal/mol was obtained. HOMO-LUMO analysis and quantum theory of atoms in molecules calculations were explored to provide further insight into the reaction. The energy gap for the final product was 0.249 eV indicating a stable molecule possible to participate in other reactions. The stability was supported by average rho and Laplacian of 0.253 and -0.558, respectively via QTAIM analysis.



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P16: Development and use of novel ligands for selective separation of Co^{2+}, Ni^{2+}, and Mn^{2+} by solvent extraction via inner sphere coordination

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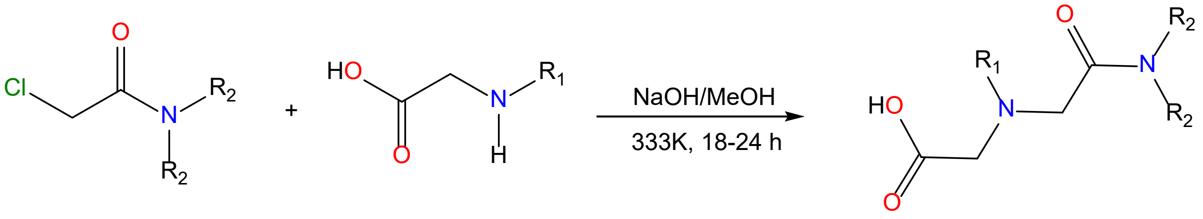
Keywords: amic acid type ligands, solvent extraction, inner-sphere coordination.

In recent times, there has been a significant rise in the demand for cobalt, particularly in the battery industry. This surge can be attributed to the growing market for portable electronic devices like smartphones, tablets, laptops, and the emerging electric vehicle sector. Despite efforts to find substitutes for cobalt in batteries, it is presumed that cobalt will remain a crucial raw material in the battery supply chain. Over the past two years, there has been a 450% increase in cobalt demand and prices. Given that cobalt is relatively expensive compared to other battery components, there is a strong focus on recovering it through battery recycling, which is important both environmentally and economically.

In the quest for more effective and environmentally friendly recycling processes for lithium-ion batteries (LIBs), in this study we investigated novel amic acid-type ligands derived from amino acids. These ligands aim to improve the separation of nickel (Ni) and cobalt (Co) from manganese (Mn) metal ions through solvent extraction. One such ligand, referred to as **L2**, featuring a methyl group on the central nitrogen atom, exhibited high selectivity for Co over Ni and Mn within a short 5-minute extraction period. Interestingly, over a longer duration, the selectivity shifted towards Ni over Co and Mn. These ligands hold promise for cobalt recycling from spent batteries, contributing to the establishment of a resource recycling society. This approach could help reduce the amount of hazardous materials destined for landfills and lessen dependence on mineral resources.



R_1: H, Methyl, ethyl, and isobutyl

R_2: Octyl / Hexyl

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P17: Synthesis of metal-organic framework and ternary quantum dot composites as electrochemical sensor for the detection of bisphenol A

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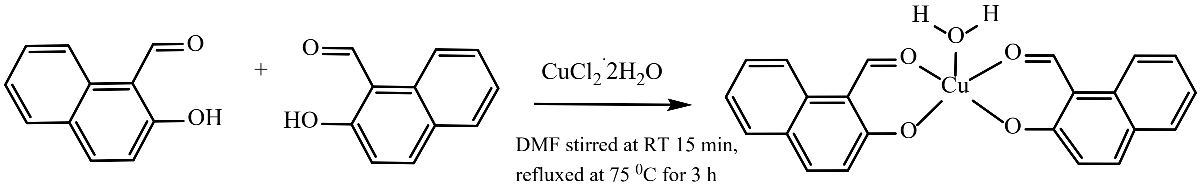
Keywords: Bisphenol A, metal-organic framework, electrochemical, composite

The manufacture of epoxy resins and polycarbonate plastics uses bisphenol A (BPA), an endocrine disrupting chemical (EDCs) and a pervasive environmental pollutant that is found in many consumer goods [1]. Due to its harmful effects on human reproductive systems, it is necessary to develop sensitive and selective sensor for its determination. Several techniques are being explore but each has inherent limitations and in recent years, the use of electrochemical sensors have received considerable attention. In this study, we present, the synthesis of metal-organic frameworks (MOFs) [Cu(2-HNA)$_2$(H$_2$O)], ternary quantum dots (TQDs) and their composite as electrochemical sensors to determine BPA. The results obtained from the studies revealed that the composite is very sensitive and selective for the determination of BPA compared to MOFs and TQDs separately, and its florescence intensity was enhanced in the presence of the analyte. FTIR, UV-Vis, single crystal X-ray crystallography, SEM and TEM, EDX were the various spectroscopic and electron microscopy techniques employed to characterize the precursors before and after usage. The composite modified electrode shows precise responses with a low detection limit of 4.70 ηM and limit of quantitation of 14.26 ηM over a broad concentration range of 10 – 50 ηM (S/N=3) ($R^2 = 0.999$). This technique because of its selectivity and sensitivity may be adapted for the detections of other hazardous endocrine disrupting chemicals.



Scheme 1: Synthesis of MOF [Cu(2-HNA)$_2$(H$_2$O)]

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P18: Biogenic synthesis of silver nanoparticles and their interaction studies with bovine serum albumin

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Keywords: silver nanoparticles, bovine serum albumin, Senecio madagarensis, fluorescence.

The synthesis of metal nanoparticles can be accomplished through the use of biogenic synthetic technique [1,2]. In this study, an environment-friendly method was used to prepare aqueous leaf extract as bio-reducing and capping agent. A change in colour in the reaction mixture, and surface plasmon resonance (SPR) band appearance at 411– 415 nm in the absorption spectra confirmed the synthesis of silver nanoparticles (AgNPs). Powder XRD patterns confirmed the phases as face-centred crystal structure of metallic silver. TEM micrograph revealed that the AgNPs were spherical and polydisperse with decreasing particle size as the concentration of the silver salt increases with particle size in the range 13 – 25 nm. The optical band gaps for AgNPs prepared with 20 mM were 2.71, 2.73 for AgNPs prepared with 50 mM and 2.66 eV for AgNPs prepared with 100 mM. The SEM-EDX confirmed the presence of elemental Ag. The results show that *S. madagascariensis* served as an environmentally friendly bioactive agent for the preparation of silver nanoparticles. For most of the AgNPs, data obtained from the BSA electronic spectrophotometric titrations showed significant hyperchromic shifts which indicate an unwinding of the protein strands [3]. Fluorescence data indicated that static quenching played a role in the formation of the complex between AgNPs and BSA [4].

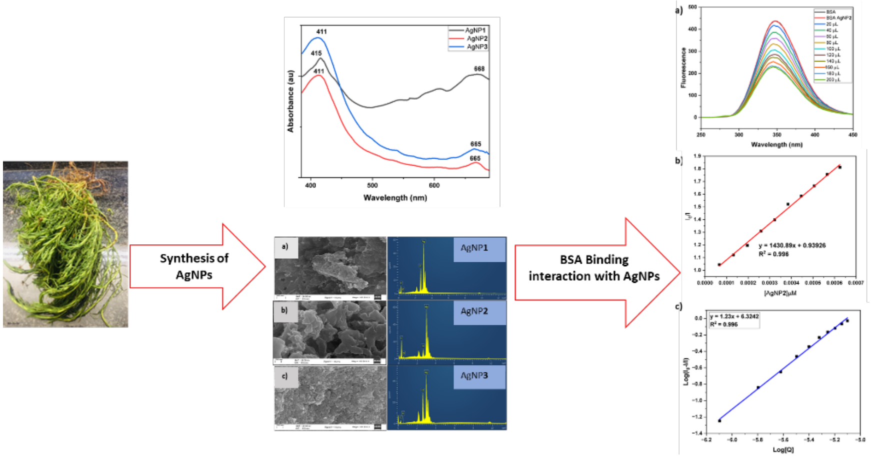

Figure 1: The synthesis of silver nanoparticles using *S. mada* plant extract and BSA interaction.

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P19: Copper(II) complexes derived from naphthalene-based halogenated Schiff bases: Synthesis, structural analysis, DFT studies and biological activities

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Keywords: Schiff base, metal complexes, crystal structure, DFT, biological activities

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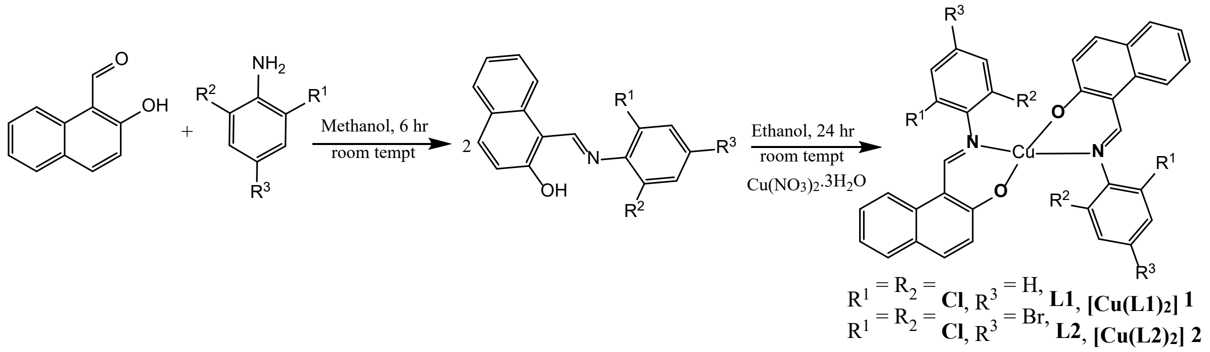
Two Halogenated Schiff bases namely, (E)-1-(((2,6-dichlorophenyl)imino)methyl)naphthalen-2-ol (**L1**) and (E)-1-(((4-bromo-2,6-dichlorophenyl)imino)methyl)naphthalen-2-ol (**L2**) were synthesized and reacted with copper(II) nitrate trihydrate in ethanol to give Cu(**L1**)$_2$ (**1**) and Cu(**L**$_2$)$_2$ (**2**). All the ligands and complexes were successfully characterized using FT-IR, UV-Vis, ^{1}H & ^{13}C-NMR as well as mass spectra. Electron paramagnetic resonance (EPR) was used to confirm the paramagnetic nature of **1** and **2**. Furthermore, the single X-ray crystal structures of **1** and **2** were determined, confirming the formation of mononuclear species in which the Cu(II) center was bonded to two bidentate Schiff bases (**L1** or **L2**) adopting a slightly distorted square planar geometry. Density Function Theory studies revealed that, complex **2** with lowest energy band gap (ΔE) of 2.49 eV is the most reactive among the compounds. α-Amylase and α-glucosidase assays were used to evaluate the antidiabetics potential of the compounds. Complexes **1** and **2** displayed very promising antidiabetic activities with IC$_{50}$ values of 148.126 mM and 107.786 mM for α-amylase assay while it was 171.559 mM for acarbose (reference drug). The antioxidant potential of the compounds was investigated using nitric oxide (NO), ferric reducing ability power (FRAP) and 2,2-diphenyl-1-picrylhydrazyl (DPPH) assays. The compounds showed moderate to good antioxidant activities with **1** and **2** having IC$_{50}$ values of 100.044 mM and 247.463 mM for NO scavenging assay, which relatively surpass Vanillin with IC$_{50}$ value of 466.626 mM. All the compounds showed poor to moderate results against *Escherichia coli*, *Staphylococcus aureus*, *Bacillus substilis*, and *Pseudomonas aeruginosa*. However, none of them were active against *Klebsiella pneumoniae*. Generally, **1** and **2** displayed better antidiabetes, antioxidant, and antibacterial potential than **L1** and **L2**.



Scheme 1: Synthesis of Schiff bases **L1** and **L2** and their Cu(II) complexes **1** and **2**.

P20: Copper(II)-photocatalyzed hydrocarboxylation of Schiff bases with CO_2

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The escalation of atmospheric carbon dioxide (CO_2) concentrations, propelled by human activities, has emerged as a key driver of global warming [1, 2]. Over the period spanning from the advent of the Industrial Revolution in 1750 to 2019, CO_2 levels soared from 280 ppm to 415 ppm, prompting governments worldwide to implement measures aimed at reducing emissions. Among these measures, the concept of recycling CO_2 into valuable products has gained prominence. Nonetheless, CO_2 poses significant challenges due to its exhaustively oxidized carbon centre and linear structure, resulting from the delocalization of its lone pairs of electrons over each adjacent C=O π bond, thereby endowing it with remarkable chemical stability. Consequently, promoting C−C bond-forming reactions via CO_2 incorporation typically necessitates strongly reductive conditions [3].

One promising approach to convert CO_2 into valuable chemicals and secondary energy sources is through homogeneous transition metal catalysis. However, most transition metal catalysts used in this process involve rare, expensive, and potentially harmful metals such as ruthenium, rhodium, palladium, and iridium. These metals are often chosen for their strong absorption, long excited state lifetimes, and high redox potentials. In contrast, copper presents a compelling alternative. Abundantly available in the earth's upper crust, copper offers several advantages. Not only does it possess low toxicity, but it also exhibits significant potential as a photocatalyst. Its abundance and favourable properties make it an attractive candidate for catalytic applications aimed at CO_2 conversion [4].

In this study, we synthesized and evaluated two copper complexes, Cu(II)-Byp and Cu(II)-BypMe, to investigate their photocatalytic hydrocarboxylation properties using a series of synthesized Schiff bases as substrates. Employing mild reaction conditions (room temperature, 1 atm CO_2, Blue LED light), we achieved yields of unnatural α-amino acids ranging from 5% to 44%. Additionally, we performed in vitro studies on both the hydrocarboxylation products and their respective precursors to evaluate their antimicrobial and antifungal activities. This investigation aimed to assess the potential application of the synthesized compounds as agents against microbial and fungal pathogens [5].

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P21: Metalate anion extraction for separation of cobalt(II) from nickel(II) and manganese(II)

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Keywords: Solvent extraction, hydrometallurgy, lithium-ion batteries

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Metalate anion extraction is a type of solvent extraction that relies on the interaction between hydrophobic cations in a water immiscible solvent and anionic metal complexes in aqueous solution. The extractant is often a neutral species such as an amine which can be protonated when brought into contact with an acidic solution. The overall process is depicted in the figure below. The anionic metal species, for example a chlorido metalate $[MCl_x]^{y-}$, encounters the positively charged extractant at the solvent interface where they can form an ion pair through non-contact interactions such as hydrogen bonding. This transfers the metal complex to the organic phase from where it can be stripped by a slightly basic aqueous solution which deprotonates the ligand and releases the metal to the aqueous layer. The attractiveness of this form of solvent extraction for separation of Co(II) from Ni(II) and Mn(II) lies in the fact that Co(II) can form $[CoCl_4]^{-2}$ in chloride solutions whereas for Ni(II) and Mn(II), this species is not observed and exists mainly in cationic or neutral form.

My presentation will briefly mention the different forms of solvent extraction with a more detailed focus on metalate anion extraction and its applicability for separation of Co(II) from Ni(II) and Mn(II) as a means of recycling NMC battery cathodes. I will report on some research which has been done in this field for my PhD thesis which focusses on the use of diamines rather than the conventional monoamines used in industry. I will discuss some of the successes the project has brought about as well as some challenges which were encountered. Finally, I will conclude with the outlook for this research and suggest where improvements may be possible.

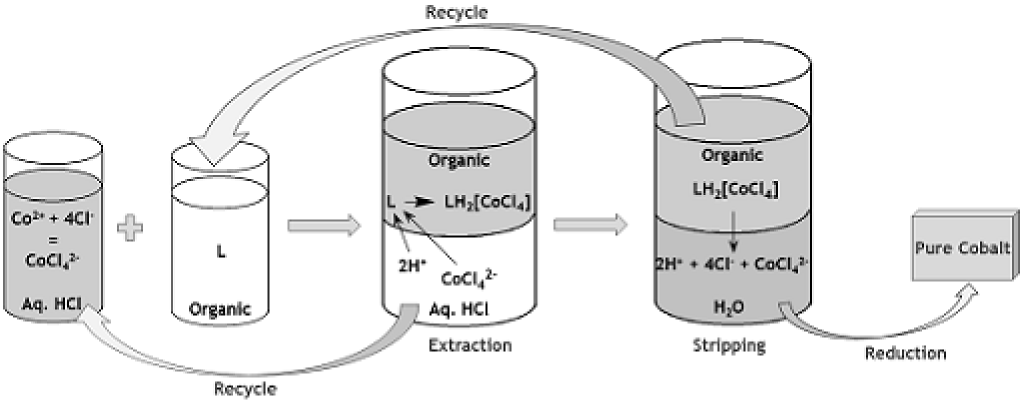

Figure 1: Overview of metalate anion extraction of cobalt(II) from aqueous HCl solution.

P22: Utilization of reduced graphene oxide intercalated Mn/Co bimetallic system for poly matrix pollutant electrodetection

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Keywords: 2,4-dichlorophenol, Bimetalic, electrochemical impedence

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A highly paramagnetic bimetallic ensemble intercalated with pi electron rich system of reduced graphene oxide was synthesized and characterized by Fourier transform infrared spectroscopy, ultraviolet-visible spectroscopy, cyclic voltammetry and electrochemical impendence spectroscopy. When used as an electrode modifier, the system exhibited high electron transfer ability/low resistance to charge transfer as confirmed by cyclic voltammetry and electrochemical impedance spectroscopy respectively. The cobalt oxide, manganese oxide graphene oxide ensemble was utilized as a glassy carbon electrode modifier and applied on 2,4-dichlorophenol as a test analyte in both its pure form and in the presence of a range of other compounds with which it is commonly found in both industrial effluent and in the environment. The detection platform was found to be very favourable towards the test analyte as evidenced by spontaneous oxidation Gibbs energy of 25.34 kJ mol^{-1} K^{-1}, an up to 80% pollutant tolerant level and high resistance to fouling.

P23: Synthesis of graphene oxide-gold nanorods nanocomposite-porphyrin conjugate for improved dual cancer phototherapy performance

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Keywords: graphene oxide; gold nanorods; TMePyP; photothermal; singlet oxygen; cytotoxicity

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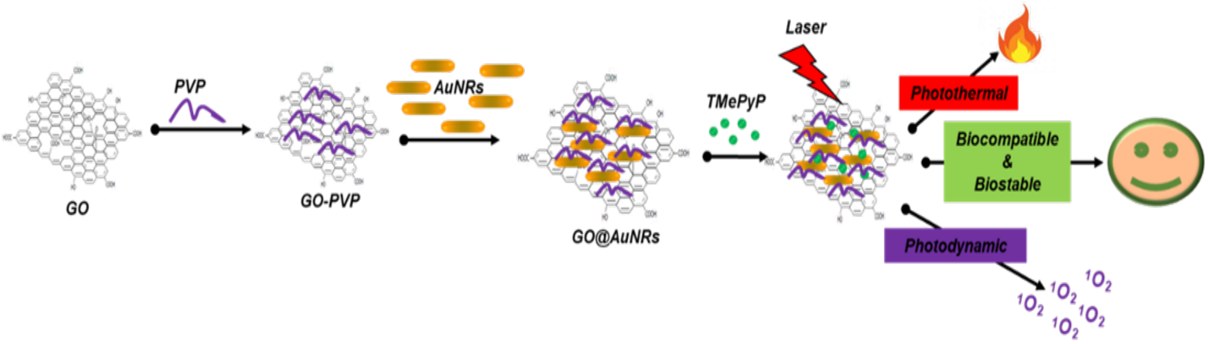
The cancer mortality rate has increased, and conventional cancer treatments are known to have many side effects. Therefore, it is imperative to find a new therapeutic agent or modify the existing therapeutic agents for better performance and efficiency. Herein, a synergetic phototherapeutic agent based on a combination of photothermal and photodynamic therapy is proposed. The phototherapeutic agent consists of water-soluble cationic porphyrin (5,10,15,20-tetrakis(N-methylpyridinium-3-yl)-porphyrin, TMePyP) and gold nanorods (AuNRs) anchored on graphene-oxide (GO) sheet. The TMePyP was initially synthesised by the Adler method, followed by methylation, while GO and AuNRs (absorbing at 850 nm, with an average size of 36.60 × 5.96 nm) were synthesised using Hummer's and seed-mediated methods, respectively. The structural and optical properties of TMePyP were confirmed using UV-Vis, zeta analyser, PL, FTIR and NMR. The TMePyP had five typical porphyrin peaks, with a zeta potential of +31.25 mV and emitting at 661 and 708 nm. TMePyP and AuNRs were anchored on GO to form GO@AuNRs-TMePyP nanocomposite, which showed reduced emission due to GO and AuNRs absorption. Nonetheless, the as-synthesized nanocomposite was stable in RPMI and PBS medium and, on irradiation, produced higher heat than the bare AuNRs, with high photothermal efficiency. In addition, the nanocomposite had higher singlet oxygen than TMePyP with high biocompatibility in the absence of light. These results indicated that the as-synthesized nanocomposite is a promising dual photodynamic and photothermal agent for cancer therapy.



Scheme 1. Schematic illustration of the preparation and properties of the GO@AuNRs-Porphyrin conjugate.

P24: The effect of different stabilisers on stability and photothermal profiling of gold nanorods

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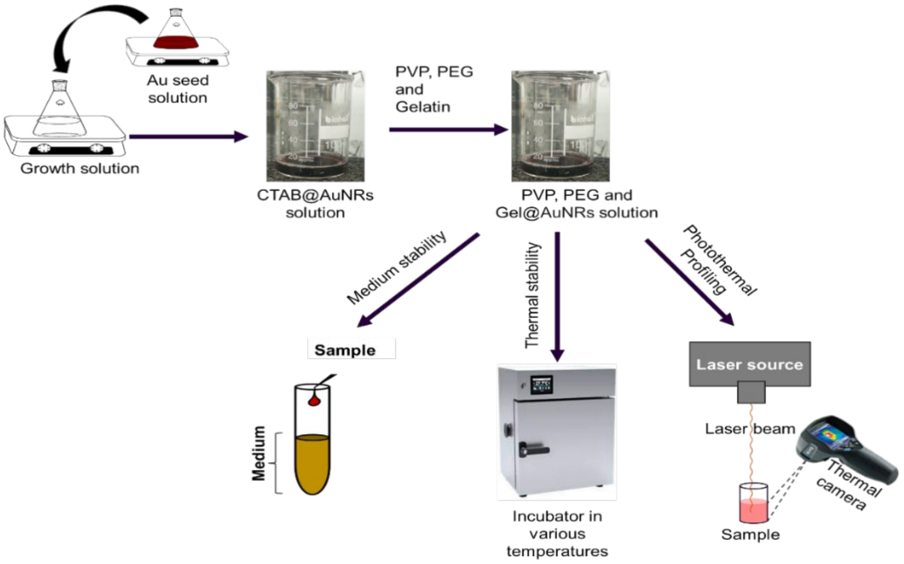
Keywords: gold nanorods; surface modification; PVP; PEG; gelatin; stability

Gold nanorods (AuNRs) have unique optical, photothermal, and biological properties that make them a popular photothermal agent. The properties of AuNRs are due to the longitudinal and transverse surface plasmon resonances (LSPR and TSPR) that they produce [1]. However, the biotoxic compound used to synthesise AuNRs limits their biological applications. As a result, researchers have sought to remove the stabiliser used during synthesis and coat them with different polymers [2]. Despite this, a comparative study on the effect of different stabilisers on the thermal and medium stability of AuNRs has not yet been conducted. Therefore, this study reports a comparative investigation of thermal and medium stability of AuNRs coated with polyvinylpyrrolidone (PVP@AuNRs), polyethylene glycol thiol (PEG@AuNRs) and gelatin (Gel@AuNRs). The stability of the as-synthesized coated AuNRs was evaluated in two commonly used cell culture mediums: the Roswell Park Memorial Institute 1640 (RPMI-1640) and Dulbecco's phosphate-buffered saline (PBS) using UV-Vis-NIR and dynamic light scattering. The as-synthesised coated AuNRs were more stable in the PBS medium than in the RPMI medium. All the coated AuNRs showed good thermal stability at 50 °C. The PEG@AuNRs generated the most heat compared to the PVP@AuNRs and Gel@AuNRs. This study demonstrated the successful coating of AuNRs with PVP, PEG, and Gelatin and their prospective usage as a photothermal agent in photothermal therapy.



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P25: Crystal structure, Hirshfeld surface analysis and antiproliferative activities of ruthenium and osmium complexes with tropolonate ligands

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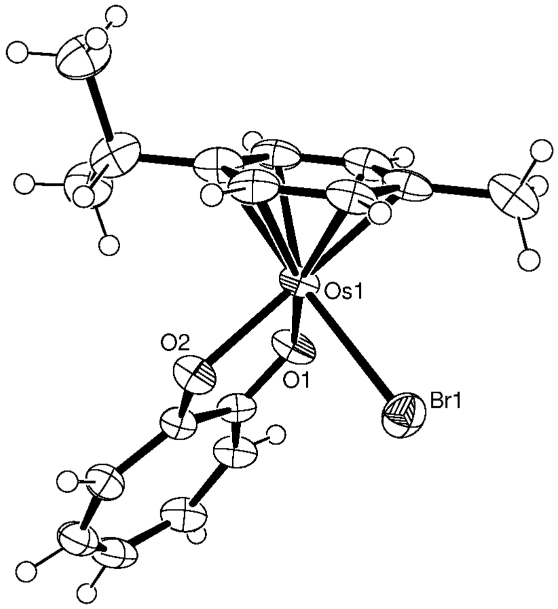
Keywords: Osmium, ruthenium, tropolone, antiproliferative.

Transition metal complexes with chelating O-donor ligands such as β-diketones are well-known and have been studied extensively, however, their biological properties, such as antiproliferative activity, have only recently become the focus of several bioorganometallic studies. Ruthenium complexes have been shown to exhibit lower toxicity and have different mechanisms of action compared to the platinum drugs currently used in chemotherapy. Alternatively, organometallic osmium complexes have been shown to exhibit interesting antiproliferative properties similar to or better than their ruthenium analogues.[1]

Tropolone ligands and their derivatives exhibit interesting physicochemical properties such as fungicidal, antibacterial, insecticidal, antitumour and neuroprotective activities.[2] The general mechanism of action for tropolone ligands is targeting of cell membranes which increases permeability leading to cell lysis.

Tropolone-based complexes exhibit numerous unique features such as forming the stable five-membered chelate rings with metal centres, and planar seven-membered π-system.[3] This study reports the crystal structures, Hirshfeld surface analysis, protein docking and antiproliferative activities of half-sandwich ruthenium and osmium complexes with tropolonate ligands.



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P26: The integration of acid leaching with metal-organic framework-based adsorption for the efficient extraction of platinum group metals

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Keywords: Metal-Organic framework, Platinum Group Metals, extraction, separation

Platinum group metals (PGMs) play a crucial role in various industries, from automotive catalytic converters to electronics manufacturing[1]. However, traditional extraction methods often pose environmental challenges and are not always economically feasible. One approach gaining attention is the integration of acid leaching techniques with Metal-Organic Framework (MOF) based adsorption. Acid leaching, particularly with hydrochloric acid (HCl), has emerged as a robust method for releasing PGMs from complex matrices like phosphogypsum (PG)[2,3]. By optimizing leaching conditions, researchers have achieved significant improvements in PGM recovery rates. On the other hand, MOFs, engineered with specific ligands, have shown remarkable selectivity in capturing PGM ions. These tailored MOFs enable targeted extraction and separation of PGMs from complex mixtures. What sets MOFs apart is their scalability and recyclability, making them ideal for large-scale PGM recovery operations[4]. By integrating acid leaching with MOF-based adsorption, we seek to overcome some of the challenges associated with traditional extraction methods. In our research, we focus on refining the integration process, exploring some novel MOFs, and finally assessing their practicality for industrial-scale implementation in PGM extraction processes. By adjusting the concentration of the leaching agent, temperature, duration of the leaching process, and the solid-to-liquid ratio parameters, we aim to maximize the efficiency of the leaching process, enhance recovery, and improve the efficiency and sustainability of resource extraction operations.

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P27: Functionalised graphitic carbon nitride nanohybrids for the piezoelectric-photocatalytic degradation of organic contaminants in wastewater

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Keywords: graphitic carbon nitride, photocatalysis, piezoelectric, wastewater treatment

At present, South Africa is faced with the brunt of the energy crisis, with the second most ubiquitous concern being water scarcity. As the most imperative renewable energy on Earth, solar energy is termed inexhaustible; however, its use is limited in numerous energy conversion technologies. Furthermore, the utilisation of solar energy in the field of photocatalysis is far from prevalent. The use of graphitic carbon nitride (g-C_3N_4) in photocatalysis has gained much popularity due to its photodegradation mechanism, visible-light-response, band structure, stability, low price, easy preparation, and innumerable potential applications. This research aims to advance the engineering of g-C_3N_4 by fabricating heterostructures with diverse morphologies to improve the efficacy of visible-light-driven photocatalytic activity for eliminating emerging organic pollutants in wastewater.

Bulk g-C_3N_4 is limited by insufficient sunlight absorption, low surface area and fast recombination of photo-induced electron-hole pairs [1]. The formation of heterojunctions containing metal/non-metal g-C_3N_4, in addition to varied morphologies such as nanoflowers, nanorods, nanowires, and nanotubes, enhance the visible-light photoactivity of g-C_3N_4-based catalysts. The coupling of wide-band-gap inorganic semiconductor oxides with doped metal/non-metal g-C_3N_4 is beneficial based on their energy band levels in promoting the separation of photoexcited electron-hole charges [2].

The preliminary objective of this study proposes to explore the potential of synthesised visible-light-driven ZrO_2@P-doped g-C_3N_4-based nanoflower composites for its use in piezoelectric-photocatalysis (PEPC). The use of PEPC (Figure 1) is hypothesised to promote synergistic effects in such complex heterostructures, highlight charge transfer pathways, alleviate high electron-hole recombination, and address constant improvement in light absorption for reduction in bandgap [3].

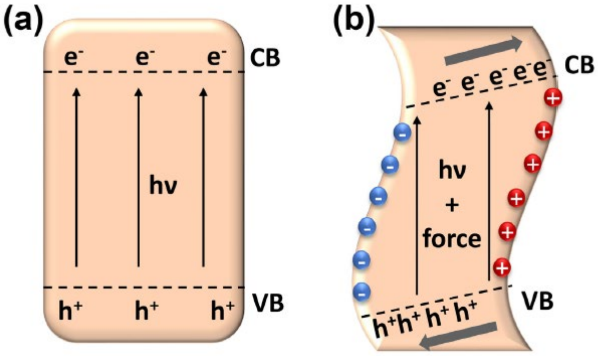

Figure 1: Mechanism of PEPC: (a) photocatalysis and (b) piezoelectric-photocatalysis [3]

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P28: Towards anticancer studies: Redox-mediated interactions of dansyl-based diruthenium complexes with biological molecules, GSH and ROS

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Keywords: redox-induced cancer cell death, diruthenium complexes, chemotherapy

Reactive oxygen species (ROS) and glutathione (GSH) are small molecules in tumorigenic cells that aid to induce cancer cell death in chemotherapy. ROS, produced during cellular respiration, instigate oxidative stress in the cells which is curbed by the anti-oxidant GSH in order to maintain the cellular redox homeostasis. The disruption of the interactions between these two biological targets are reported to tigger various types of cell death pathways (e.g. apoptosis, ferroptosis, etc.) due to an imbalance in the cellular redox environment.[1] Metal-containing anti-cancer drugs interact with the biological reducing agent GSH due to their redox-active metal centre. As such, these have been considered for research focus in redox-mediated cancer cell death mechanisms.[2] The topologies as well as the synergistic anti-cancer activities of bimetallic ruthenium complexes with non-steroidal anti-inflammatory drugs (NSAIDs) of diruthenium complexes has led to the investigation of these metal-metal bonded complexes as anti-tumour agents.[3] In this project, novel mixed-ligand diruthenium complexes, $[Ru_2(O_2CCH_3)_3(Rap)(DsIm)_n]Cl$ where R = 2,4-$(CH_3)_2$, 4-CH_3, 2-F, 4-F substituents on an anilinopyridinate (ap) ligand and n = 1 or 2 (**C1** – **C4**) , were synthesised and decorated axially with a biologically-active dansyl-imidazole (DsIm) ligand. One-electron metal-centred oxidation ($Ru_2^{5+/6+}$) and reduction ($Ru_2^{5+/4+}$) processes were observed for these dansyl-imidazolium complexes through cyclic voltammetry and spectroelectrochemical characterisations. These Ru_2^{5+} complexes were found to bind to GSH reducing agent with binding constants in the range of $10^7 – 10^{10}$ M^{-1}, followed by a reduction to Ru_2^{4+} which results in the production of the oxidised disulphide GSSG. A cell-free dichlorofluorescein (DCF) assay showed that the dansyl complexes can also be oxidised to Ru_2^{6+} in the presence of hydrogen peroxide while generating hydroxyl radicals as ROS. Upon screening the diruthenium complexes against the MCF-7 breast cancer cell line, they all exhibited cytotoxic properties against the tumorigenic cells. Moreover, the bis dansyl-imidazolium complex (**C4**) was found to be the most potent as benchmarked against cisplatin[4] at 100 µM concentration after 72 hours of incubation.

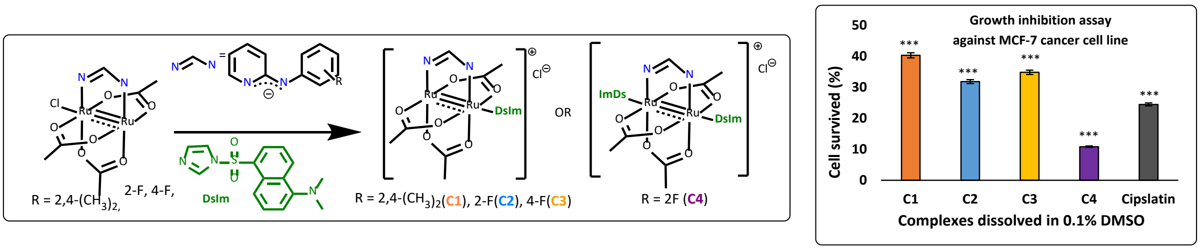

Figure 2 Novel dansyl-imidazolium complexes and their biological screening against the MCF-7 breast cancer cell line.

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P29: Synthesis and characterisation of *meso*-substituted pyrrole-based metal complexes as potential DNA binders

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Keywords: dipyrromethene, copper complex, crystal structure, DNA binding, viscosity, gel electrophoresis.

Transition metal complexes as potential anti-cancer therapeutics is an exciting, growing field of research. Several N-donor ligands have shown promising anti-cancer activity when complexed to transition metals. [1] These metal-complexes are reported to have a variety of biological targets with DNA being a major target.

Bilirubin (a heme metabolite) typically forms metal complexes through its dipyrromethene moieties (Fig 1a). A study conducted on a bilirubin Cu(II) complex reported strand breakages and cleavage of calf thymus DNA.[2] Ruthenium complexes that had the same dipyrromethene motif (with meso-substituents) were reported to bind to DNA via an intercalative mechanism and displayed significant cytotoxicity.[3]

In this study a series of copper dipyrromethene complexes, that contain varying substituents on the phenyl ring located at the *meso* position (Fig 1b), were synthesised and characterized by standard spectroscopic techniques. The structure of the complexes was confirmed by single crystal X-ray diffraction (XRD).

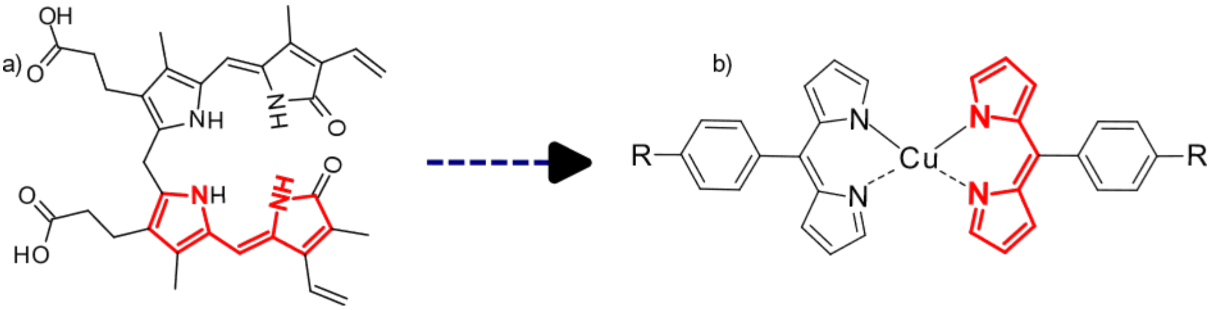

Figure 1: (a) structure of bilirubin with the dipyrromethene motif highlighted in red; (b) general structure of the *meso*-substituted dipyrromethene complexes synthesised where R represents the substituent to be varied and the dipyrromethene motif highlighted in red.

The binding affinity of the complexes to DNA were then investigated by UV-vis titration of calf thymus DNA into a buffered solution of the complex. The potential mode of DNA binding was then further investigated by a range of techniques including UV-vis spectroscopy, viscosity measurement, agarose gel electrophoresis and molecular docking studies. Overall, the complexes were found to bind to DNA via an intercalative mechanism.

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P30: Synthesis and characterization of water-soluble nanoparticles and their application in fluorescence imaging

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Keywords: Quantum dots, nanoscience, sensing, selectivities.

Herein, we report an aqueous synthesis of zinc selenide using water-soluble precursors under ambient conditions. The prepared zinc selenide nanoparticles were capped with thioglycolic acid (TGA) which allows for controlled nucleation of particles and prevents exponential growth. The formation of the nanoparticles was confirmed by FTIR, XRD, UV, PL, SEM, and TEM. The UV showed a peak at 380 nm, which is blue-shifted compared to the bulk material, the blue shift is attributed to the quantum confinement effect which is common to all nanosized materials. FT-IR confirmed the adsorption of thioglycolic acid on the surface of the ZnSe surface (Zn^{2+}) surface. The XRD pattern suggests the cubic phase crystal structure of the prepared nanoparticles, further confirming the presence of the nanostructured materials. The particles are stable in water for 12 days until they precipitate. The photoluminescence spectrum showed a broad emission peak at 430 nm. The prepared particles were labeled with target-specific ligands to promote cellular uptake and showed efficient cell uptake into cell nuclei making them potential candidates for drug delivery to cell nuclei.

P31: The synthesis, X-ray characterization, spectroscopic and Hirschfield surface analysis of dimeric metal centers featuring phenacyl-esters

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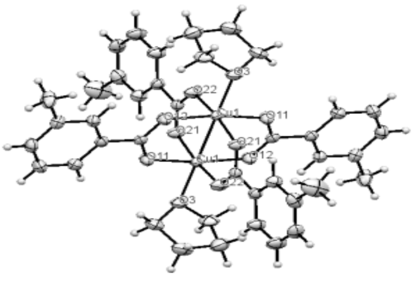
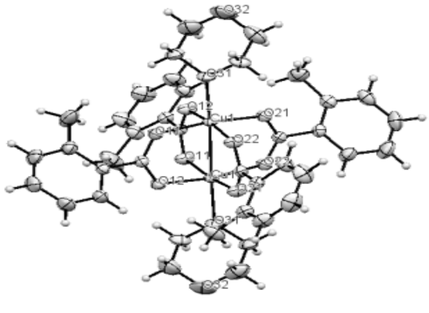
Keywords: Copper paddlewheel, phenacyl-esters, single-crystal XRD crystallography, supramolecular assembly, Hirshfield Surface Analysis

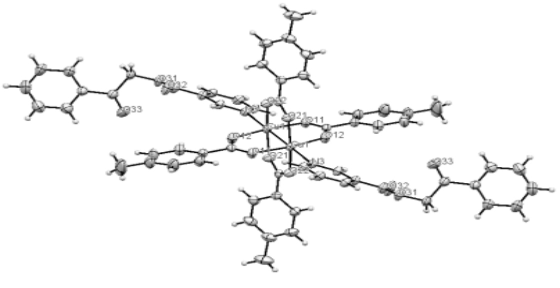
In this study, the synthesis and characterization of carboxylate paddlewheel copper complexes were investigated and reported. The complexes consist of O -, and N- donor ligands which coordinated in the apical positions of the copper (II) paddlewheel complexes. The primary focus was the investigation of the influence of the incoming substituent on the structure; more especially with regards to the spectral properties and thermal properties of the synthesized compounds. Synthesized complexes ranged from simple mononuclear complexes; dinuclear dimers; supramolecular 1D networks and a tetranuclear copper (II) compound.

Characterization of complexes was done using analytical, and spectroscopic techniques such as single crystal diffraction analysis, FT-IR spectroscopy, thermal analysis and Hirschfield surface analysis. The series of dinuclear paddlewheel complexes obtained with ligands (L = THF **(1)**, C_4H_8O **(2)**, $C_{14}H_{11}NO_3$ **(3)**) revealed a square pyramidal geometry with the methyl-substituted phenyl carboxylate groups bridging the two copper atoms in a syn-syn coordination mode. Extended supramolecular complexes were synthesized via the reaction of three synthesized structurally bifunctional organic ligands and the tetrakis(μ-carboxylato-O,O)dicopper(II) core.

Compounds synthesized include:







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P32: Antimicrobial activity of rhenium(I) tricarbonyl 2-(pyridin-2-yl) quinoline complexes coordinated with various azoles

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Keywords: Antimicrobial agent, Azoles, Quinoline, Rhenium(I)

The increase in antimicrobial resistance and lack of effective drugs to fight against resistant strains have become a serious problem for public health [1]. Rhenium(I) tricarbonyl complexes have demonstrated their great potential as antimicrobial, anticancer, and most recently, anti-COVID agents [2]. This study involves the synthesis of quinoline-based ligands and their analogues Re(I) complexes. The *fac*-[Re(CO)$_3$(2-pyridin-2-yl-quinoline)(H$_2$O)] intermediate complexes are used to coordinate various azole ligands (i.e., pyrazole, imidazole, and imidazole derivates) for anticancer and antimicrobial applications. The synthesised ligands and complexes were characterized using single-crystal XRD, FTIR, ^{1}H and ^{13}C NMR, and UV/Vis. Figure 1 shows the crystal structures of (a) 2-pyridin-2-yl-quinoline and (b) *fac*-[Re(CO)$_3$(2-(pyridin-2-yl) quinoline)(Pz)] as seen in Figure 1, which crystallized in the monoclinic system, and in the P2$_1$/*n* and P2$_1$/*c* space groups respectively.

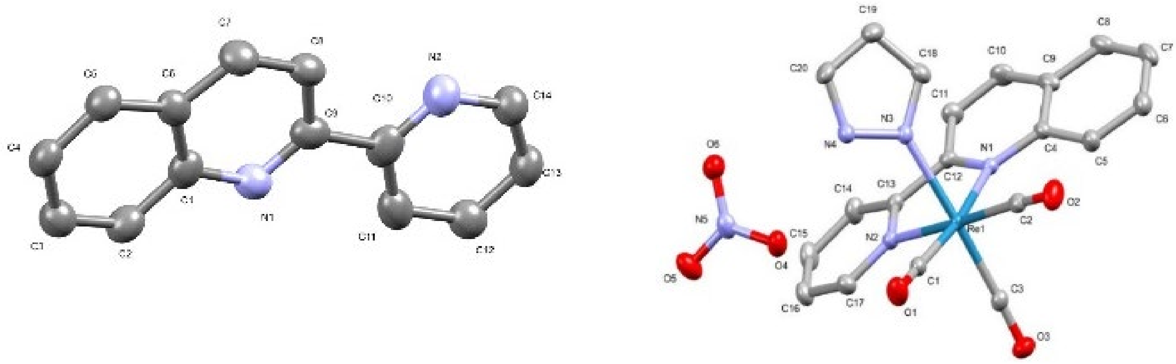

Figure 1 Single crystal X-ray structure of the (a) 2-(pyridin-2-yl) quinoline and (b) *fac*-[Re(CO)$_3$(2-(pyridin-2-yl)quinoline)(Pz)]; Pz = pyrazole.

The antimicrobial activity of the 2-(pyridin-2-yl) quinoline ligand and seven (7) Re(I) complexes of the form *fac*-[Re(CO)$_3$(2-(pyridin-2-yl) quinoline)X)]; where X = H$_2$O; Imidazole; 1-CH$_3$ Imidazole; 2-CH$_3$ Imidazole; 1,2-Di-CH$_3$ Imidazole; Pyridine and Pyrazole, was determined against *C. alblican, S. aureus, E.coli, S. pyogenes, P. aeruginosa.* Most of the complexes displayed antimicrobial activity at a minimum inhibitory concentration (MIC, µM) of ≤ 0.075, which according to the literature is classified as acceptable for antimicrobial agents [3].

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P33: Solventless synthesis of cation-doped 2D-$CoSe_2$ nanomaterials for water splitting and supercapacitance

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Keywords: Cobalt diselenide, water splitting, 2D nanomaterial, molecular source precursors.

The global energy crisis is of serious concern lately, due to the rapid depletion of fossil fuels which are predominantly used in electricity power generation. Researchers have been searching for alternative sustainable energy generation and storage technologies. One of the solutions towards this is the development of hydrogen energy and next-generation supercapacitors, which mostly incorporate nanomaterials as the main active component. Among other categories, two-dimensional (2D) nanomaterials are desirable for these tasks due to their structural stability and large surface areas suitable for electrochemical processes. This study has focused on transition metal dichalcogenides (TMDCs) 2D nanomaterials [1], which are analogous to and outperform graphene [2]. We report an easy and simple preparation technique for pristine and metal doped $CoSe_2$ TMDC nanomaterials. The synthetic approach is mainly a low-temperature, solventless thermolysis of the corresponding phosphine-free transition metal selenobenzoate complexes. The crystallographic, morphological and microelemental information of the fabricated 2D nanomaterials were confirmed by pXRD, TEM and SEM-EDX. The nanomaterials were found to exhibit interestingly efficient electrocatalytic activities towards hydrogen generation through water splitting reactions, as well as good supercapacitance behaviour.

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P34: Synthesis, characterisation and anticancer activity of pyrazole-based ruthenium(II) arene complexes

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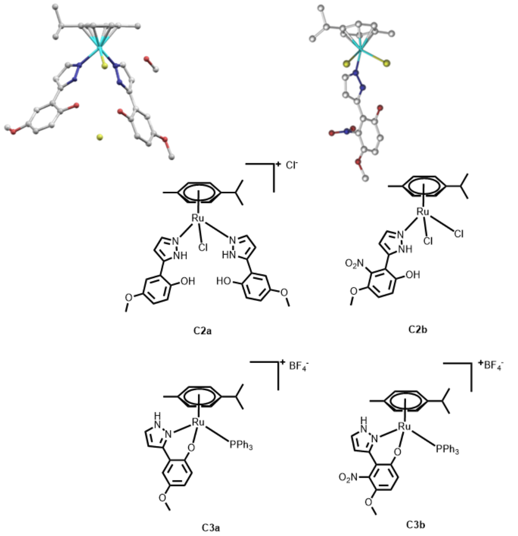
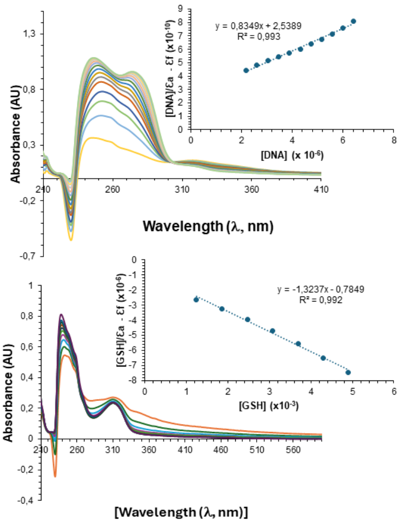
Keywords: pyrazole, ruthenium, DNA, cancer

Pyrazole containing molecules exhibit a broad spectrum of activity, including anti-microbial, anti-fungal and anti-cancer properties.[1] The advent of platinum group metals (PGMs) as metallodrugs unlocked a new perspective towards cancer treatment and has garnered widespread success in the field of medicinal chemistry. Ruthenium emerged as suitable candidate due to the ability to access several oxidation states that are further accessible under physiological conditions. The ability ruthenium to mimic the binding of iron to transferrin, a glycoprotein involved in iron transport, allows for the selective accumulation of Ru(II) in the hypoxic cancerous environment.[2] Furthermore, the inert η^6-arene moiety on Ru(II) complexes stabilises the biologically active Ru(II) metal center from rapid oxidation and confers hydrophobic properties that enhance cellular accumulation.[3]





In this study we evaluate the dependence of the biological activity on the substituents present on the pyrazole ligand of these pyrazole-based ruthenium(II) arene complexes. These novel complexes were synthesised and characterised as to their, spectroscopic and electrochemical properties. The x-ray structures herein presented, reveal the ligand-to-metal ratio preferences of the Ru(II) arene complexes based on the basicity of the pyrazolyl ligand. Preliminary screening of the complexes in breast cancer cell lines, *i.e.* MCF-7, T47D and the highly aggressive MDA-MB-231 shows cell line-specific activity with reduction of cell viability. The complexes show minimal selectivity for non-cancerous cells (MCF-12A), supporting ruthenium's favourable selectivity properties. Titrations of the complexes with salmon sperm DNA were monitored using UV-visible absorption spectroscopy and show interaction with DNA with binding constants in the order of 10^5 M^{-1}. The complexes were shown to bind to glutathione (GSH), a reactive oxygen species (ROS) quencher, with binding constants in the order of 10^2 - 10^3 M^{-1}.

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P35: Novel *ansa*-bis(indenyl) ligands for transition metal complexes: synthesis and characterisation

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Keywords: indenyl, titanium, ansa ligand.

The interest in transition metal sandwich complexes with indenyl ligands is still very high in synthetic organometallic chemistry [1]. Indenyl substituted derivatives are of great interest because of their multiple applications in catalytic polymerization processes, as well as a potential source of bioactive compounds in metallopharmaceuticals [2-3].

A series of *ansa* bis-indenyl functionalized sandwich complexes of group 4 transition metals (titanium, zirconium and hafnium) will be explored for biological activity. The synthesis of the ligands was achieved by the low temperature lithiation of indene, followed by the addition of phenylphosphonic dichloride or 1,2 dibromoethane to afford the *ansa*-ligand. The products were isolated as either oils or solids in medium to high yields and have been preliminary characterised using NMR and FT-IR.

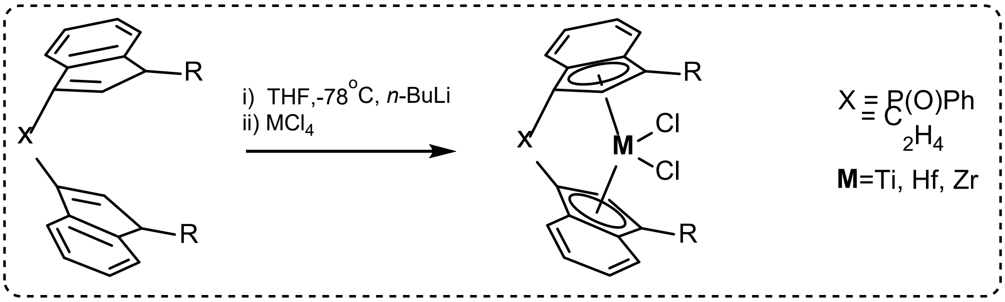

Figure 3: Proposed ansa-bis(indenyl) complexes of Group IV transition metals

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P36: Application of deep eutectic solvents as extraction media for azeotropes

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Keywords: DESs, Azeotropes, Thermophysical properties, Liquid-liquid extraction, Activity coefficient at infinite dilution.

The research into deep eutectic solvents (DESs) is comparatively in its infancy, with a first discovery of DESs made in 2001 by Abbott et al. [1]. They are usually obtained by the complexation of a quaternary ammonium salt with a metal salt or hydrogen bond donor (HBD) and are known as systems formed from a eutectic mixture of Lewis or Brønsted acids and bases which can contain a variety of anionic and/or cationic species [2]. By carefully choosing the components of these vicennial solvents, it is possible to achieve a nontoxic and biodegradable solvents. Most DESs are easy to synthesise and do not react with water and are acknowledged as a new class of ionic liquids (ILs) analogues due to similarities in physical properties between DESs and ILs. In this study different types of DESs were prepared and characterised using different techniques and their separation efficiency for azeotropic mixtures was determined using Gas-Liquid Chromatography and Liquid-Liquid Equilibria. The results were correlated using NRTL, Othmer-Tobias and hand correlation equations.

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P37: Synthesis, structural, morphological and optical characterization of gC_3N_4/ZnO as a potential photocatalyst

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Keywords: Graphitic carbon nitride ($g\text{-}C_3N_4$), ZnO, heterojunction photocatalyst, metal oxide

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Graphitic carbon nitride ($g\text{-}C_3N_4$) and metal oxides such as ZnO have recently become the most widely used materials in the field of photocatalysis. This is because of their remarkable properties, which include low cost, biocompatibility, chemical inertness, and excellent thermal and photostability. However, these two semiconductors have drawbacks of high charge recombination rate, limited specific surface area, and insufficient use of visible light. Attempts have been made to circumvent these drawbacks using a wide range of photocatalytic enhancement techniques, such as coupling with other semiconductors to form heterojunctions.

In this study, graphitic carbon nitride was functionalized with ZnO nanoparticles to enhance its photocatalytic efficiency. The gC_3N_4 was prepared by the calcination method and exfoliated, while spherical-shaped ZnO nanoparticles were prepared by a facile solvothermal method using Zn(II) dithiocarbamate complex as precursor complex and ethyleneglycol as surfactant. The effects of different calcination temperatures (600 and 750 ºC) on the crystallinity, elemental composition, morphological, and optical characteristics of the nanocrystalline gC_3N_4/ZnO was investigated using different analytical techniques.

The X-ray diffraction patterns revealed the formation of a highly crystalline hexagonal structure of wurtzite ZnO nanoparticles with an increase in the degree of crystallinity as the calcination temperature increased. Microscopic analysis of the surface and internal morphologies indicated that the nanoparticles were made up of nanospheres with an average diameter of about 15 nm, which increased with temperature due to the self-assembly from smaller nanocrystallites triggered by high temperature that enhanced their surface reactivity. Remarkably, the spherical morphology of these self-assembled nanospheres was well preserved despite the high temperature calcination process. Optical measurement showed that the band gap energy of the ZnO nanoparticles decreased from 3.24 to 3.14 eV with an increase in calcination temperature from 600 to 750 °C. The results from the nano-compositing of the gC_3N_4 with ZnO showed improvement in both the surface area and electronic structure of the resulting semiconductor heterostructures. Therefore, this study presents an alternative perspective on the functionalization of $g\text{-}C_3N_4$ with ZnO, which produced a heterojunction system with potential for use in photocatalytic applications.

P38: CuO nanoparticles functionalised graphitic carbon nitride for the degradation of ibuprofen in water

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Keywords: Water treatment; photocatalysis; pharmaceuticals; ibuprofen; nanoparticles

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The increase in the consumption of pharmaceuticals and personal care products (PPCPs) has led to their wide detection in different water matrices including lakes, wetlands, and rivers. In this study copper oxide (CuO) nanoparticles incorporated into graphitic carbon nitride were investigated as photocatalyst for the efficient degradation of ibuprofen under UV light irradiation. The obtained nanocomposites were characterized for their physiochemical, optical, and electronic properties using different analytical techniques. Evaluation of the photocatalytic efficiency of the nanomaterial showed an enhancement in the activity of the composite, which was attributed to improved charge carrier property of the composite. The CuO/g-C_3N_4 achieved about 85.6% degradation efficiency of Ibuprophen, which was used as a model pharmaceutical pollutant, compared to 71.48 and 57.89% achieved by the pristine g-C_3N_4 and CuO respectively. The composite also showed a composition dependent efficiency, with an improvement in activity observed as the percentage composition of CuO was increased. This was attributed to the improved light absorption and reduced recombination process that were significant for enhancing the ibuprofen degradation. Evaluation of radical species showed that $^{\bullet}OH$ was the most significant radical species for ibuprofen degradation. A study of the charge transfer mechanism in the composite, showed that the p-n heterojunction at the composite's interface, led to improved charge transport and separation that also contributed to the effectiveness of the material. The stability of the material after about 4 cycles of reuse also confirmed that this nanocomposite holds high potential for application in wastewater treatment.

P39: DFT calculations of Ag doped MoS_2 nanocomposite biosensor for highly sensitive detection of pathogens

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Keywords: Ag/MoS_2, density functional theory, sensors, nanocomposites

Escherichia coli, known as E. coli, is a species of bacteria. Some E. Coli strains can cause illness, however the majority of strains are benign and aid in the everyday functioning of the digestive system. One important development in the field of food safety is the use of biosensors for the identification and detection of foodborne illnesses. In order to identify the presence of particular compounds, biosensors are analytical tools that combine a biological component (such as enzymes, antibodies, or microbes) with a physicochemical detector [1,2]. Compared to conventional culturing methods, they have a number of benefits that address some of the drawbacks that indicated. Chalcogenide-based nanomaterials (molybdenum disulphide) have been modified to improve the detection of E. Coli has been receiving much attention. Herein, a novel highly sensitive Ag/MoS_2 nanocomposite has been developed and simulated using density functional theory (DFT) to demonstrate the mechanism for improved pathogen detection. Simulations show the band structure, electrical and optical properties indicate that incorporating of Ag atoms improves the detection capability of MoS_2. Furthermore, the findings demonstrate a theoretical framework for Ag atom adsorption on the MoS_2 2D structure to enhance the conductivity of MoS_2 nanosheets, hence supporting the potential applications of this structure.

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P40: Supercritical carbon dioxide synthesis of iron-based metal organic frameworks

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Keywords: Metal-organic framework, supercritical carbon dioxide, Acid mine drainage waters

Supercritical carbon dioxide ($scCO_2$) method has gained vast amount of interest in nanomanufacturing of various chemicals, pharmaceuticals, in food and fabric industries. This method intends to replace organic solvents with inexpensive, nontoxic, nonflammable CO2. $scCO_2$ is beneficial for synthesis of metal-organic frameworks (MOFs) due to unique properties such as the inability to condense, low viscosity, and high diffusion rates [1]. It is worth noting that many polar molecules and molecules with large molecular weight have poor solubility in CO_2 thus making it a challenge on synthesis of MOFs. CO_2 is a poor solvent due to the lack of dipole moments, insufficient dielectric constant and low polarizability per unit volume [2]. To overcome this challenge, co-solvents ($scCO_2$ and organic solvents) that can dissolve both polar and nonpolar substances are added [3]. Reported here is the synthesis of Fe-MIL-88B and Fe-MIL-101 employing acid mine drainage waters (AMD) as the source of iron (Fe) and waste polyethylene terephthalate as the source of terephthalic acid (H_2BDC). The prepared materials were comparable to those prepared via the conventional solvothermal reactions. Fourier transform and powder X-ray diffraction confirmed the coordination of BDC to Fe metal clusters. The results of nitrogen adsorption showed that micro- and mesopores predominate in both materials, which is advantageous for hydrogen adsorption. The MOFs break down at temperatures higher than 400 °C demonstrating the materials' thermal resilience. This work has revealed that scCO2 can be used to synthesize these Fe-MOFs.

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P41: Optimum route for the preparation of activated zeolitic imidazolate framework-derived carbons for CO_2 adsorption

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Keywords: CO_2 adsorption, activated carbon, zeolitic imidazolate framework, surface area, porosity, adsorption capacity

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Carbon dioxide (CO_2) is one of the leading greenhouse gasses emitted in combustion of fossil fuels for power generation. It is prominently contributing to the catastrophic changes in climate change and global warming. The CO_2 emission levels in the atmosphere are increasing daily and that has encouraged researchers to develop sustainable innovation technologies to attenuate it. Adsorption is the promising technology, however, finding an adsorbent with high CO_2 adsorption capacity and selectivity is still a significant challenge. Zeolitic imidazolate frameworks (ZIFs) are a sub-family of metal-organic frameworks (MOFs) which are highly recognized due to their facile transformation into porous carbons, and additional advantages such as tunable structural, physicochemical, and targeted textural properties. Herein, a range of ZIF-derived carbons (ZDCs) were successfully produced through the carbonization process of ZIF-8 and cellulose acetate (CA) using four different routes. The respective activated forms of ZDCs were also successfully synthesized using potassium hydroxide (KOH) as an activating agent. All the prepared samples were analyzed using characterization techniques such as Fourier transform infrared (FTIR) spectroscopy, powder X-ray diffraction (PXRD), thermogravimetric analysis (TGA), Raman spectroscopy, Brunauer-Emmett-Teller (BET) analysis, and scanning electron microscopy (SEM). The activated ZDCs revealed a different morphology compared to the parent (ZIF-8). The BET analysis proved that KOH introduction creates a rich microporous structure resulting in a great improvement in the specific surface area as 2191 m^2/g was obtained as the highest surface area. Propitiously, the enhanced surface area and porosity led to high CO_2 adsorption capacities. Furthermore, ratio variation between the ZIF-8 and CA was done from 1:10 to 5:10 molar ratio, to optimize the carbons adsorption capacity and efficiency. Therefore, these activated carbons are promising as adsorbents for CO_2 capture.

P42: Structural, morphological and spectroscopic properties of magnetite quantum dots: Effects of temperature and time

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Keywords: Magnetite, quantum dots, band gap

The unique sizes, shapes and crystalline phases of nanomaterials determine their potential applications [1]. Quantum dots have shown good efficacy as diagnostic and therapeutic agents as well as photocatalysts for environmental remediation and solar fuel energy [2-5]. Magnetic quantum dots have an extra advantage in different applications due to their magnetic properties that enable magnetic targeting. In this study, a solvothermal method in a conventional reflux setup was followed in the preparation of magnetite quantum dots under nitrogen gas [6]. Effects of temperature and time on the structural, morphological and spectroscopic properties were investigated. Powder X-ray diffraction patterns of the iron oxide quantum dots were used to identify the crystalline phase as magnetite regardless of the reaction parameters. Transmission electron microscopy (TEM) images showed spherical shapes with average particle sizes of 3.25, 3.3 and 3.90 nm for reaction temperatures of 200, 180 and 165 °C respectively, and this shows increasing particle size with decreasing temperature. In the investigation of the effect of time, reaction times of 3 and 6 h resulted in the same mean particle size of 3.25 nm while a bigger mean particle size of 7.5 nm was observed for a reaction time of 4.5 h. Despite the different parameters employed in the syntheses of these nanoparticles, the mean particle sizes within the range of 3-8 nm were observed and they can therefore be referred to as quantum dots. The optical spectra of the quantum dots showed maximum wavelengths of 200-210 nm. The optical band gap increased with increasing reaction temperature, with band gaps of 5.01, 5.13 and 5.49 eV for temperatures of 165, 180 and 200 °C. Reaction times of 3 and 6 h resulted in the same optical band gap of 5.44 eV whereas a reaction time of 4.5 h resulted in a bandgap of 3.75 eV. Fourier transform infrared spectra confirmed the capping of the quantum dots with oleate.

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P43: A physicochemical investigation of the mechanism of formation of Cu_2S in insulation materials in liquid-filled transformers

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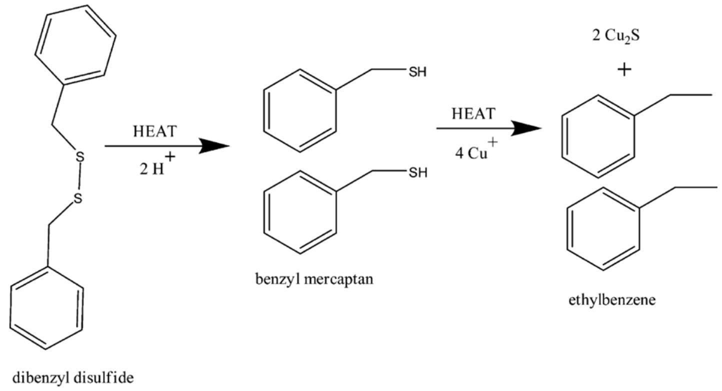
Keywords: dibenzyl disulfide (DBDS), copper sulfide, transformer oil

This study is based on insulation materials used in fluid-filled, high and low power voltage transformers, and the monitoring and adaption of these materials to reduce insulation failure. Fluid-filled transformers are commonly insulated with Kraft cellulose-based paper and mineral transformer oil [1]. However, both components are influenced by ageing that can be due to oxidative, thermal and electrical stresses.

Apart from this, corrosive sulfur components in the oil also become hazardous (they eventually form copper sulfide) to the copper windings, paper and oil insulation itself. Research has shown that the most common causative agent of corrosive sulfur is dibenzyl disulfide (DBDS), which is used as an anti-wear agent in transformer oil [2]. The pathway for copper sulfide formation is believed to be via the formation of a DBDS-Cu intermediate that eventually leads to the deposition of copper sulfide on the windings (influencing their conductivity) and in the oil and paper (influencing their ability to function efficiently as a dielectric) [3].

This study showed an alternative pathway for copper sulfide formation. In Scheme 1, dibenzyl disulfide cannot oxidatively or reductively adsorb onto copper surfaces, however, the degradation products of dibenzyl disulfide, namely, benzyl mercaptan and dibenzyl sulfide can. This in turn forms a thiolate complex that can degrade to form copper sulfide. Thiolate formation seems plausible as it was also synthesized in a transformer oil matrix [4].



Scheme 1: Proposed mechanism for the formation of Cu_2S on transformer copper windings by Leeward and Reed.

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P44: Development, optimization and performance of a novel reactor for acid mine drainage remediation using batches of natural substrates

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Keywords: acid mine drainage, natural substrates, passive treatment, adsorption

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This paper discusses the development, optimization and performance of an innovative reactor designed for the passive treatment of acid mine drainage (AMD) using natural substrates. Acid mine drainage (AMD), a widespread environmental concern caused by effluents from mining operations, is typically marked by acidic water and high levels of dissolved toxic ions and heavy metals. AMD poses significant risks to the ecosystem and the environmental integrity, potentially leading to the ecological devastation of watersheds and the pollution of surface water bodies.

In this paper, state-of-the-art analytical techniques and instruments mainly FTIR, SEM-EDS, XRF, and XRD were used for the characterization of materials. Ion Chromatography was employed to determine anions such as SO42-. The ICP-OES and ICP-MS were used for the analysis of metals and metal ions.

The metal content (Fe^{3+}, Mn^{2+}, Cr^{2+}, Cu^{2+}, Ni^{2+}, Pb^{2+}, Al^{3+}, and Zn^{2+}) and anions contained in AMD matrices were effectively removed, achieving high removal efficiencies. Therefore, this novel technique has proven to be effective in treating AMD from mining activities. This technique could benefit the mining industry by providing an affordable wastewater treatment technology with very low operational costs and minimal energy consumption. Additionally, the possibility of recycling and reusing AMD water in operations offers further reductions in operational costs.

P45: Synthesis of Fe_3O_4 and silica-supported N^O chelating agents towards the removal of Cd(II), Cr(VI), and Pb(II) cations from aqueous solutions

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Keywords: chelating agent, magnetic nanoparticles, MCM-14, SBA-15, extraction, metal cations.

Heavy metal pollution of water is one of the most challenging environmental concerns to human and aquatic life [1]. As such, several technologies have been developed to remove heavy metal cations from water bodies [2]. This study focused on the synthesis of N^O organic ligands and immobilization on Fe_3O_4, MCM-41, and SBA-15 for the extraction of Cd(II), Cr(VI), and Pb(II) cations from aqueous solutions (**Fig. 1**). The Schiff base ligand 2-(((3-(triethoxysilyl) propyl) amino) methyl) phenol (**L2**) was immobilized onto magnetic nanoparticles and silica material to yield the **L2@Fe_3O_4**, **L2@MCM-41** and **L2@SBA-15** chelating agent. The immobilized material was characterized using FT-IR, ^{1}HNMR, SEM, TEM, EDX, PXRD, BET, VSM, and TGA-DTA/DSC techniques. Extraction of the cations using the chelating agents was investigated under optimized conditions of pH, contact time, initial concentration, and adsorbent dosage to give removal efficiencies of >97%. The adsorption kinetics followed pseudo-second-order models, while equilibrium data was most effectively described by the Freundlich isotherm model. The extraction mechanism of the metal cations occurred through electrostatic interactions.

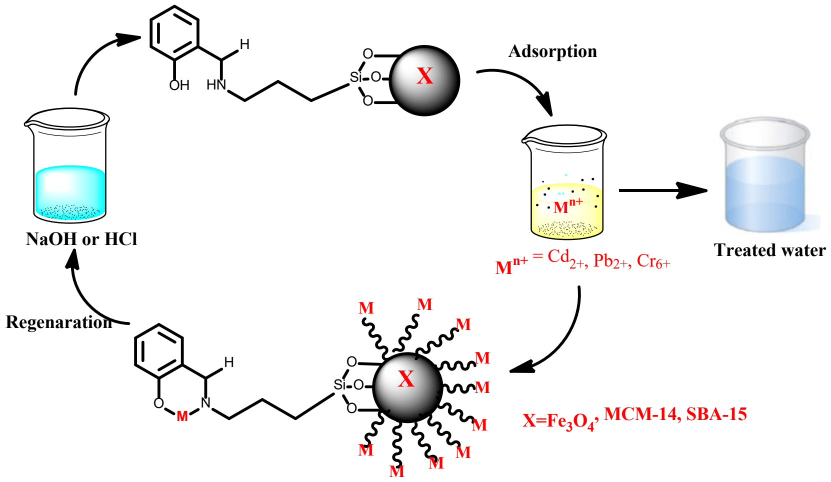

Fig 1. Extraction of metal cations using Fe_3O_4 MNPs, MCM-41, and SBA-15 immobilized on N^O chelating agents.

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P46: Synthesis and photocatalytic performance of $Ag_3PO_3/ZnFe_2O_4$ composite on tetracycline in water

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Keywords: Photocatalysis, wastewater, zinc ferrite, silver phosphate, tetracycline

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Antibiotics are one of the most commonly consumed drugs in the pharmaceutical industry. Specifically, tetracycline (TC) as a model antibiotic has been reported to be the most used antibiotic drug in the world. Despite its importance and efficiency in human treatment, the abuse of TC could be deadly, and its toxicity could contaminate surface water. TC is extremely difficult to effectively remove from water using conventional treatment methods. Therefore, research interest has continued to increase in developing effective methods and materials to efficiently remove TC from water. The use of novel heterogeneous catalysts to improve the oxidation rate and degradation efficiency of tetracycline at mild operating conditions could be an efficient route. In this study, $AgPO_3$-$ZnFe_2O_4$ heterojunction semiconductor nanocomposites were synthesized at different ratios using hydrothermal processing in conjunction with in-situ precipitation. This composite combines the characteristics of both silver phosphate and zinc ferrite, offering enhanced functionalities that neither material possesses individually. The performance of nanocomposite was explored for the complete mineralizing of TC in wastewater.

The phase structure, composition, morphology, and optical properties of the nanocomposites were assessed by X-ray diffraction, Energy dispersive X-ray spectroscopy, Scanning electron microscopy, Transmission electron microscopy, and UV-vis spectroscopy. The effect of process parameters such as the solution pH, initial concentration of tetracycline, and catalyst dosage were evaluated. The photocatalytic degradation results showed that the $AgPO_3$-$ZnFe_2O_4$ (1:1) achieved a high degradation efficiency within 60 min of reaction, compared to the pristine Ag_3PO_4 and $ZnFe_2O_4$. The assessment of radical scavenging reactions indicated that the process of degradation proceeded hugely via a non-radiative process. Furthermore, the nanocomposites were found to be reusable for up to 4 cycles without a significant loss in their efficiency. This study showed that the $AgPO_3$-$ZnFe_2O_4$ (1:1) could be a potential and reliable catalyst for the degradation of tetracycline from wastewater.

P47: Water electrolysis for green hydrogen production using metal organic frameworks

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Keywords: green hydrogen, water electrolysis, metal organic framework, electrocatalysis

In the transition of energy source from fossil fuels to renewables, the green Hydrogen production plays a major role and hydrogen economy being the energy driver of the future in mitigating the effects of carbon emission [1,2]. In this study, we perform the water electrolysis which is a route for hydrogen production using metal organic frameworks (MOFs) as electrocatalysts. Two different metals, M_1 and M_2 were chosen to produce three MOFs containing M_1-MOF, M_2-MOF and M_1-M_2-MOF. The MOFs prepared were characterized using powder X-Ray diffraction, infrared spectroscopy. The morphologies visualized using scanning electron microscopy revealed spherical structures for M1-MOF while M2-MOF revealed structured flakes. However, M1-M2-MOF showed the formation of pointed spindles dispersed with spheres indicating a synergistic interaction between the two metals used in the MOF preparation. Each of the three electrocatalysts were individually characterized using cyclic voltammetry. Water electrolysis performed on a catalyst coated membrane revealed that an onset potential of 1.380 V current densities of 1.6 mA/cm^2 at 2 V. The current study will further showcase the stability and the kinetics of the hydrogen evolution reaction for the studied electrocatalysts.

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P48: 1D/3D PANI/WS_2 composite for highly selective room temperature sensing of ammonia vapours

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Keywords: selective, heterojunction, ammonia, room temperature

Highly selective room temperature sensors are crucial in the detection of ammonia gas for effective environmental management and non-invasive early diagnosis of diseases. The n-type WS_2, with its layered structure presents a large surface-area- to -volume ratio and a significantly large number of exposed active edge sites for maximum adsorption of gases [1]. Meanwhile, polyaniline (PANI) is a p-type highly conductive polymer that can operate at low temperatures [2]. In this study, 3D WS_2 nanoflowers were coupled with 1D PANI nano-connected fibres for improved gas sensing performance. PANI was synthesized using oxidative polymerization while a colloidal method was followed to synthesize WS_2. Subsequently, the two were used to form the PANI/WS_2 composite ex-situ.

The properties of the PANI/WS_2 composite based sensor were evaluated for their sensing performance at room temperature. The composite showed high selectivity towards ammonia compared to interferents such as toluene and chlorine. Enhanced response to the ammonia vapours compared to pure PANI and WS_2 was also observed. The improved gas sensing performance is attributed to the increased electron depletion due to the formation of p-n junction (heterojunction).

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P49: Synthesis and study of novel organometallic carbazole derivatives as heat shock protein inhibitors for malaria

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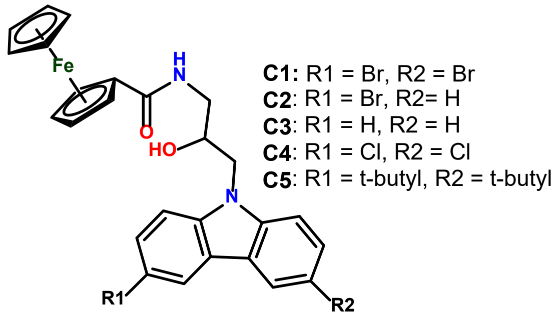
Keywords: *P. falciparum*, cancer, carbazole, HSP90

Malaria, a disease caused by plasmodium parasites, continues to be a global health challenge affecting 85 endemic countries [1]. Compared to 2021 there was an increase of five million cases of malaria reported in 2022 [1]. Alongside the increased number of cases, there have been reports of increased treatment resistance from *Plasmodium falciparum*, the deadliest of the malaria causing Plasmodium parasites [2]. Given these circumstances, there is a need for the development of novel, effective antiplasmodial compounds. Heat shock proteins (HSPs) are essential for the functioning of all eukaryotic cells as they are responsible for facilitating the correct folding of proteins within cells. Furthermore, HSP90 has been found to be overexpressed in the erythrocytic stage of malaria parasites, making it an attractive target [3]. Amino alcohol bearing carbazole derivatives have been found to inhibit *P. falciparum* HSP90 and have potent antiplasmodial activity [3]. As a result of these promising studies, five organometallic amino alcohol carbazole derivatives were synthesized for evaluation against *P. falciparum* (Figure 1).



C1: R1 = Br, R2 = Br
C2: R1 = Br, R2= H
C3: R1 = H, R2 = H
C4: R1 = Cl, R2 = Cl
C5: R1 = t-butyl, R2 = t-butyl

Figure 4: Synthesised ferrocenyl amino alcohol carbazole derivatives.

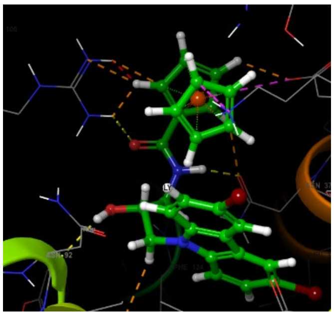


Figure 2: C1 docked into the ATP binding pocket of PfHSP90.

The synthesized target compounds were fully characterised by ^{1}H and ^{13}C NMR, FTIR and positive mode electrospray ionisation mass spectroscopy. Furthermore, their purity was determined using RP-HPLC. Computational studies were carried out using Maestro from the Schrodinger suite. Geometry optimisation of the structures was carried out at the B3LYP-D3\6-31G+* level of theory using Jaguar within the Schrodinger suite. This was followed by docking of the compounds into the N-terminal domain ATP-binding pocket of *Pf*HSP90. Docking studies revealed the compounds had potential to bind to the protein with C5 having the lowest affinity. To validate the results, *in vitro* HSP90 experiments were performed. *Pf*HSP90 expression and purification was carried out, followed by competitive binding assays using the synthesised target compounds.

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P50: Targeting breast cancer with novel organometallic complexes

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Keywords: organometallic, breast cancer, anticancer drugs, artemisinin, reactive oxygen species

Cancer is one of the leading causes of deaths worldwide and this is due to the fast rate at which cancer cells divide and grow. A current treatment for cancer is the use of platinum complexes like cisplatin or carboplatin for chemotherapy. However, these complexes have proven to be detrimental to the overall health of the patients due to the severe toxicity of these complexes on normal cells [1]. Combined with the toxicity of these complexes, drug resistance has also become a major issue which increases the need for research into new effective and less toxic anticancer drugs [2]. Drug hybrids between metal centres and known pharmacophores, such as artemisinin have been the focus of recent research. One artemisinin derivative, artesunate, is a highly effective antimalarial drug and has also shown great potential towards cancer treatment [3]. One drug target in cancer cells is the endoplasmic reticulum (ER). Cancer cells exist under heightened levels of ER stress making it possible to tip the balance to apoptosis in cancer cells by using ER stress inducing agents, while causing minimal effect to the normal cells [4]. This ER stress can be achieved by the generation of reactive oxygen species (ROS) that is a common mode of action of PGM complexes as well as artemisinin derivatives.

In this presentation, the synthesis and characterisation of organometallic PGM complexes (**Figure 1**) that contain an artemisinin moiety will be discussed. The aqueous solubility and stability of these complexes were investigated. The inhibitory effects of the complexes were also evaluated against MCF-7 and MDA-MB-231 breast cancer cell lines, and the MCF-12A normal cell line. A possible mode of action was also investigated through a ROS detection assay.

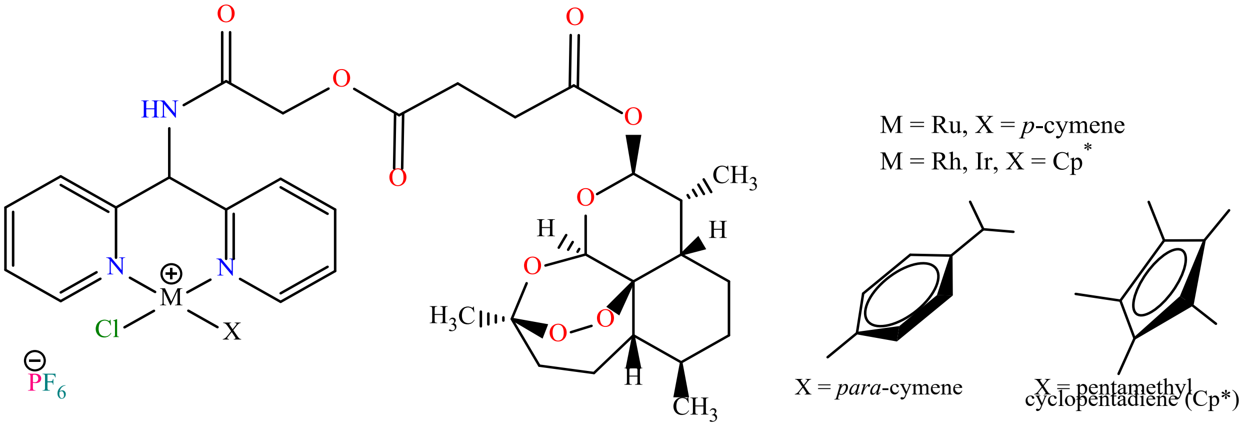

Figure 5: The organometallic complexes screened for activity against breast cancer cell lines.

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P51: Novel ferrocenyl quinoline-benzimidazole molecular hybrids as antileishmanial agents

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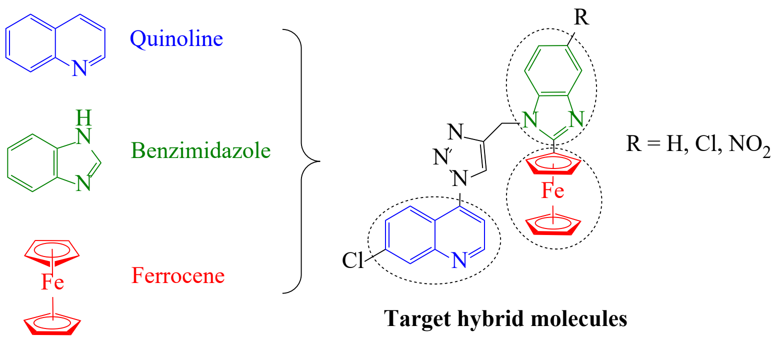
Keywords: Leishmaniasis, quinoline, benzimidazole, ferrocene, hybridisation

Cutaneous leishmaniasis, the most pervasive form of the infectious and vector-borne disease of leishmaniasis, is chiefly caused by *Leishmania major* in the developing world [1]. Patients are scarred by disfiguring, and often permanent lesions. With no efficacious vaccine available yet, therapeutic medication is the mainstay to alleviate morbidities. However, due to the advent of resistance to the current drug regimen with severe drug-induced toxicity and costly treatment, an alternative recourse is proffered by the repurposing of pharmacophoric scaffolds with known activity against other infectious parasitic diseases [2].

The quinoline and benzimidazole scaffolds are privileged pharmacophores in medicinal chemistry: The former comprises the foundation of the archetypal antimalarial drug of chloroquine, while the latter is an emerging key scaffold in anticancer and antimalarial treatment [3]. Furthermore, the incorporation of metal ions in organic compounds is a nascent and thriving strategy as it may impart additional modes of action to drugs through redox activation. This is exemplified in the enhancement of antimalarial potency by compounds containing a ferrocenyl moiety [4]. Ergo, in this research, the strategies of molecular hybridisation and metal complexation were combined to synthesise a series of ferrocenyl-derived, benzimidazole–quinoline hybrid compounds. Following stability and cytotoxicity testing, the *in vitro* antileishmanial activity of the synthesised complexes were investigated against intracellular and extracellular *L. major* parasites of the LV39 strain. *In vivo* assays using a mouse model of *Leishmania* and potential modes of action will also be presented.



Target hybrid molecules

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P52: Thermodynamics and computational study of the molecular interactions between water and imidazolium and pyrrolidinium based ionic liquids

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Keywords: Redlich–Mayer equation, apparent molar properties, solute-solvent interaction, DFT

Over an extended period, the scientific community has expressed apprehension regarding the emission of volatile organic compounds (VOCs) [1]. Research experts are actively exploring the potential of ionic liquids (ILs) as environment-friendly solvents to mitigate environmental impacts by replacing VOCs [1].

ILs are a promising alternative because of their distinctive characteristics, including chemical and thermal stability, remarkably low vapor pressure, non-flammability, and capacity to dissolve a diverse array of organic and inorganic compounds. These attributes make ILs outstanding replacements for conventional volatile solvents [2]. Therefore, the current investigation focusses on the measurement of thermophysical properties, density and sound velocity of binary mixtures containing ionic liquids 1-butyl-3-methylimidazolium thiocyanate or chloride [Bmim][SCN] or [Bmim][Cl], and 1-butyl-1-methylpyrrolidinium chloride [Bmpym][Cl] (Fig. 1) and water at different temperatures and concentration.

The primary objective was to scrutinize the influence of temperature and ionic liquid concentration on molecular interactions within these mixtures. Leveraging this data, we performed calculations to derive key thermodynamic parameters, including apparent molar volume (V_φ), apparent molar adiabatic compressibility (K_φ), limiting apparent molar expansion ($E_\emptyset^0$), and thermal expansion coefficients (αp). The application of the Redlich–Mayer equation allowed us to determine the limiting apparent molar volume (V_φ^0) and limiting apparent molar adiabatic compressibility (K_φ^0) along with their associated parameters (S_v , B_v, S_k , B_k).

Furthermore, to gain insights at the molecular level, density functional theory calculations were performed to examine the molecular interactions. This multifaceted approach provided a comprehensive understanding of the thermodynamic nuances within the ionic liquid mixtures in this study, offering valuable implications for engineering applications and process design.

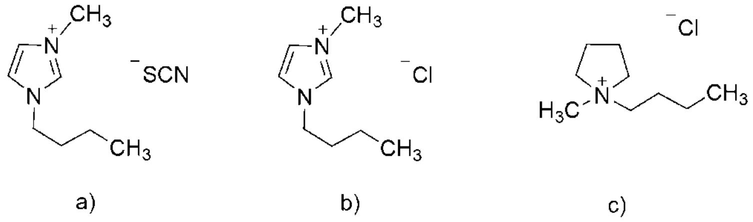

Fig. 1. Ionic liquids used in this study: (a) [Bmim][SCN]; (b) [Bmim][Cl] and (c) [Bmpym][Cl].

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P53: Adsorptive removal of dyes from an aqueous solution using UiO-66 metal organic framework

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Keywords: Adsorption, Activation, Metal Organic Frameworks, UiO-66, Bromocresol Green, Methyl Violet

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Dyes have caused significant pollution to water bodies due to their great usage in the textile, pigment and leather industries. The presence of hazardous dyes in wastewater cause disastrous effects on living organisms and the environment. The conventional technologies for the remediation of dyes from water have several bottlenecks such as high cost and complex operation. Adsorption is an effective method for eliminating colours from tainted water. The Zr-based metal-organic framework (MOF, UiO-66) was synthesized solvothermally for the removal of Methyl Violet (MV) (anionic dye) and Bromo Cresol Green (BCG) (cationic dye). The synthesized UiO-66 MOF was activated using the direct method of heating for 24hrs at 200°C. The UiO-66 MOF was characterized by XRD, FTIR and TGA. Batch adsorption studies were conducted to investigate the effects of contact time, initial concentration, pH and adsorbent dosage on the removal of MV and BCG using UiO-66. Adsorption isotherms and kinetics studies indicated that Langmuir isotherm and pseudo-second-order kinetic models provide the best models for MV and BCG adsorption onto the UiO-66 MOF respectively.

P54: Phytochemical screening of polyphenolic extracts from South African indigenous plants for inclusion in sunscreen products

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Keywords: skin cancer, sunscreens, photodegradation, photo-stabilisation, indigenous plants

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Sunscreens incorporate a combination of organic and inorganic filters to protect our skin from ultraviolet (UV) radiation. Prolonged exposure to UV radiation causes some organic UV filters to undergo photodegradation, diminishing their ability to shield users from the negative effects of UV radiation. This study aims to determine the photo-stabilisation potential of South African indigenous polyphenolic extracts on organic sunscreen absorbers. Polyphenols may prevent the photodegradation of organic filters by absorbing UV radiation, scavenging free radicals through their antioxidant properties, or facilitating energy transfer. The plants of interest are African potato, African ginger, Aloe vera, Bushman's tea, Cancer bush, Rooibos, Buchu, and Baobab. In this work, it was essential to optimise the extraction method by varying parameters such as solvents, temperature, and pre-treatment of the plant material. Variations between the extraction parameters were monitored by comparing the UV absorption spectra within the targeted range of 290-400 nm. Optimum extraction was achieved by ultrasonication of the plant material at 40 °C for four hours with 100% ethanol. The solution was processed through filtration, ethanol removal, and subsequently immersed in boiling water. The resulting aqueous solution was filtered and extracted with ethyl acetate to produce a polyphenolic extract that exhibited high UV absorption. The extracts from Rooibos, Aloe vera, and Bushman's tea exhibited the highest absorption potential, while African ginger and Baobab exhibited the lowest UV absorption. Phytochemical screening of the extracts showed the presence of saponins, chalcones, carboxylic acids, emodins, glycosides, cardiac glycosides, steroids, phenols, alkaloids, carotenoids, quinones, and anthraquinones in all extracts. Additional phytochemicals including tannins, leuconthocyanins, triterpenoids, flavonoids, phytosterols, and phlobatannins were found absent or present in extracts, except for African potato, in which all were present. The concentration of flavonoids (equivalent concentration of quercetin (ECQ)) was highest in African ginger (4.18 ± 0.36 mg g^{-1} ECQ) and lowest in Baobab (0.18 ± 0.02 mg g^{-1} ECQ). The concentration of total phenols (measured as gallic acid equivalents (GAE)) was highest in African potato (37.2 ± 0.7 mg g^{-1} GAE) and the lowest in Baobab (3.2 ± 0.3 mg g^{-1} GAE). In conclusion, South African indigenous polyphenolic extracts have thus far exhibited the potential to enhance the photostability of organic sunscreen absorbers. Extracts from Rooibos, Aloe vera, and Bushman's tea showed strong UV absorption which may potentially photo-stabilise organic filters via their ability to absorb UV radiation. Phytochemical analysis revealed a diverse array of compounds present in the extracts, with the African potato extract exhibiting the highest concentration of the various phytochemicals tested. These findings advocate for the exploration of natural sources that can enhance the efficacy of sunscreen formulations, by offering a sustainable and potentially efficacious avenue for UV protection. Further mechanistic studies are warranted to elucidate the photo-stabilization mechanisms of these extracts for their effective integration into commercial sunscreens.

P55: Isotherm and kinetics studies on the adsorption of Zn^{2+} onto biochar/graphene oxide composites

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Keywords: Zinc; biochar; graphene oxide; adsorption

The potentially detrimental impact of heavy metal pollution on public health has become a pressing environmental issue. Therefore, there is a need to remove heavy metal contamination from environmental media. In this work the feasibility of a novel biochar/graphene oxide composite as a low-cost adsorbent for the removal of Zn^{2+} from aqueous solutions was investigated. The biochar was obtained from pyrolysis of pine pallets (BCH1) and exotic plant material (BCH2). These two biochars were studied together with graphene oxide (GO) and their composites (BCH1/GO and BCH2/GO). This study describes the adsorption isotherm and kinetics studies for the removal of Zn^{2+} from aqueous solution by using the BCH/GO composites.

During the removal process, a batch adsorption technique was conducted to observe the effect of various experimental variables such as the solution pH, contact time, mass of adsorbent, initial metal ion concentration, and temperature. The adsorption capacities (q_e) of all the BCH/GO composites increased with increasing pH, contact time, and adsorbent dose. The adsorption of Zn^{2+} onto the BCH/GO composites was conducted at an optimum pH of 6 under a constant temperature of 25 °C. BCH1, BCH2, GO, BCH1/GO, and BCH2/GO had a maximum adsorption capacity of 52.92, 73.86, 52.27, 56.67, and 62.54 mg g^{-1}, respectively for the uptake of Zn^{2+}.

The equilibrium data obtained were fitted into eight isotherm models: Freundlich, Langmuir, Temkin, Redlich-Peterson, Dubinin–Radushkevick, Sips, Toth, and Khan, and the best fit model for each adsorbent was selected based on the model with the lowest sum of squared residuals (SSR). The Freundlich and Langmuir isotherms best described the equilibrium data for the uptake of Zn^{2+} by the BCH/GO composites.

Four kinetics models including the pseudo-first order, pseudo-second order, Elovich, and intraparticle diffusion models, were employed to evaluate the sorption kinetics of Zn^{2+} onto the BCH/GO composites and to identify the possible rate-determining step. The kinetics data generated for the adsorption of Zn^{2+} onto the BCH/GO composites was best described by the pseudo-second order model, indicating that this was a bimolecular process.

It was concluded that the BCH/GO composites can be used as effective and low-cost adsorbents for removing Zn^{2+} from aqueous solution, though out of all the materials, biochar from exotic plants BCH2 performs better.

P56: Synthesis and characterization of composite track-etched membranes for application in mine-waste waters

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Keywords: Nanofibers, track-etched membranes, mine-waste waters, rhodium, iridium and platinum.

Track-etched membranes (TEM) offer distinct advantages over conventional membranes and other solid supports due to their precisely determined structure and the fact that their pores sizes and thickness can be varied in a controllable manner [1]. Composite membranes were fabricated by combining the products of ion-tracking and electrospinning processes. Swift heavy ions generated from a cyclotron were used to irradiate polyethylene terephthalate (PET) polymer film to create latent tracks which were then chemically etched in an alkaline solution, to produce tracks on the membrane. Magnetron sputtering was then used to deposit titanium (Ti) on the membrane to produce PET-TM. Ligand functionalized polyacrylonitrile nanofibres (PAN-nfs), polysulfone (PSN-nfs) and polystyrene (PSRN-nfs) were directly electrospun on the Ti coated PET-TEM using an electrospinning process creating the composite membrane. These track-etched membranes with specific pore sizes were functionalized with various N and S based ligands for scavenging Pt, Rh and Ir metal anions from mine waste waters [2]. The track-etched membrane, the nanofibres and the composite membrane were characterised using SEM, TEM, TGA, ATR-FTIR and adsorption/desorption of nitrogen techniques. Mean pore size and pore size distribution was determined using electrical conductivity and small angle X-ray scattering techniques. The results confirmed the fabrication of nanofibers-coated track-etched composite membranes. Filtration studies were conducted to assess the efficiency of the uptake of the platinum group metals and invariably separate Pt, Rh and Ir from mine wastewaters.

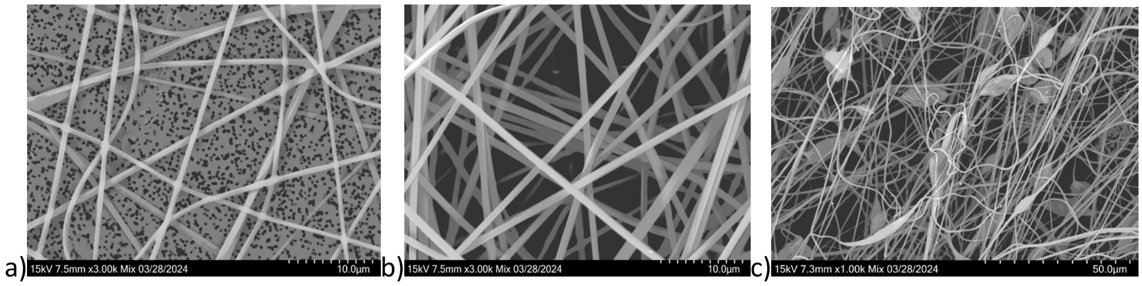

Figure 1: SEM images of the composite membranes a) Nanofibers deposited on track-etched membrane having specific pores, b) Mat of nanofibers on the track-etched membrane c) Ligand functionalized nanofibers deposited on track-etched membrane.

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