11th International Conference of the African Materials Research Society

Dec. 12 - 15, 2022



History: The African-MRS has its origins in the August 2000 'US-Africa Materials Workshop', held in Pretoria, South Africa. This Workshop, co-organized and sponsored by the United States National Science Foundation (NSF) and the South African National Research Foundation (NRF) sought to explore opportunities for collaboration between the USA and Africa with an overarching objective of developing materials research capacity in Africa. It brought together over 70 leading scientists, industrialists and government representatives from the USA and 15 African countries, which, together, sculpted a forward-looking sustainable framework for driving materials research in Africa. Building on this initiative, two years later, on 12 December 2002, the Africa-MRS was officially launched in Dakar. Subsequent biennial A-MRS ICs were held in South Africa (2003), Morocco (2005), Tanzania (2007), Nigeria (2009), Zimbabwe (2011), Ethiopia (2013), Ghana (2015) Botswana (2017) and Tanzania (2019). The conference grew steadily with time; the past three conferences have averaged over 300 participants. On the west coast of Middle Africa, Senegal is by the Atlantic Ocean to the west and Senegal River borders the country to the east and north. The capital city of Senegal, Dakar is located at the westernmost tip of the country on the Cap-Vert peninsula. Dakar is to help set the directions, including research and educational ones, across Africa. One key hope in holding this conference in Dakar is to encourage much stronger partnering between the African-MRS and counterpart organizations within Africa such that the African-MRS can diversify and grow its support network.

This year's **conference** is multidisciplinary with focus on the current and emerging materials research themes for a sustainable Africa we want, especially in the contexts relevant to Africa's development and human capacity building. As Materials outreach activities, nine (09) plenary lectures will be delivered. It is planned that the **conference** would provide a discussion platform for present and future materials challenges that would help in defining priorities and policy making for promoting sustainable materials research in the Africa this will be addressed by keynotes speakers through panel discussions. There will also be extensive public relations activities before, during and after the conference to broaden knowledge about the field and the many areas impacted by materials in Africa.

Main Themes for the conference include:

1. Materials for Mining and Manufacturing
2. Materials for Agriculture.
3. Materials for Water & Environment Monitoring.
4. Materials for Energy.
5. Biomaterials & Materials for Health.
6. Nanomaterials, Quantum Materials, Photonics Materials & Nanotechnologies.
7. Computational Materials
8. Education and Networking in Materials Science & Engineering

It is expected that the **conference activities and goals** (both general and specific) will help to develop materials science and engineering in Africa:

- Stimulate and enhance basic and applied research on materials in Africa.
- Build a network of materials researchers which encourages multi-national and multi-disciplinary collaboration in materials research specially for early careers and women scientists
- Establish scientific researchers exchange programs to allow the exchange of information and results among scientists in laboratories within Africa and abroad.
- Educate young scientists by hosting six short term schools during the conference.
- Create closer co-operation, mutual assistance and effective utilization of available and future facilities among institutions participating. Core groups would be created in the various streams of the Materials Science to plan and discuss future regional facilities.
- Improve the utilization of the available research facilities by expanding the equipment user data base. The conference will run special sessions to promote cyber-connectivity.
- Signing of Memoranda of Understandings (MOUs) among African member institutions for graduate training and sandwich PhD programs within the African and abroad.
- Develop methods to work closely with governments and state structures to improve policy and support for materials research and development
- Identify and foster specific areas of materials research as regionally appropriate
- Promote information and resource sharing, exchange and development
- Ensure that materials research contributes significantly to the various national strategies for social equity and poverty alleviation in a constructive and sustainable manner
- Encourage downstream materials manufacturing and value-adding activities
- Strengthen the resources for materials science education at all levels
- Transform leading African participants into a much more active Africa-MRS Networking Committee to oversee follow-up in research, education, exchanges, publications and joint research, and future partnering within Africa and internationally.

We express our great pleasure to invite you as a Speaker/Delegate to the 11th International Conference of the African Materials Research Society (AMRS2022), December 12-15, 2022 at the University Cheikh Anta Diop of Dakar, Dakar, Senegal.



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Prof Balla DIOP NGOM
Lead Organizer AMRS2022



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AMRS2022
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AMRS2022 WORKSHOPS

11TH INTERNATIONAL CONFERENCE OF THE AFRICAN MATERIALS RESEARCH SOCIETY

" PRE-CONFERENCE WORKSHOPS "

Date: 10 -11 December 2022
Venue: University Cheikh Anta Diop of Dakar

COACH WORKSHOP

Professional Career Development
Empowering Women in Africa to be Leaders in Science and Technology through Career Advancement Opportunities.

FACILITATORS



Dr Pushpalatha Murthy

Michigan Technological University, USA"
Email: ppmurthy@mtu.edu



Prof Abdelaziz El Jazouli

University Hassan II of Casablanca, Morocco.
Email: eljazouli_abdelaziz@yahoo.fr

PRESENTATION OF THE WORKSHOP:

Following the success of the previous COACh workshops organized in several African countries (Morocco 2013 & 2014, Namibia 2015, Rwanda 2016 & 2018 & Ghana 2019) , another workshop on **Professional Career Development** will be organized in Senegal.

Three modules are scheduled:
1) Career Launch and Acceleration,
2) Selling Your Science: The Art of Proposal Writing (includes description of USAID-PEER Program),
3) Publishing in Peer Reviewed Journals.

WORKSHOP MODULE ABSTRACT:

1- Career Launch and Acceleration

Seeking and starting that first job as a scientist or engineer is a time of great transition and uncertainly. This workshop provides techniques necessary for an effective career launch into the job that best fits your skills and interests. This workshop module will help position you to be most effective in finding and applying for a variety of job positions, developing a tailored CV for the position and being an effective communicator in the interview whether it is by phone, web-based or in person. Additional topics include effective communication

methods for teaching and research presentations, importance of network building and finding a mentor, and developing an professional internet presence.

2. Selling Your Science: The Art of Effective Proposal Writing

This workshop provides training in effective techniques for writing proposals to gain research support for a scientific or engineering project. Topics include identifying the priorities of the agency or program solicitation, determining criteria for assessment and writing to the criteria, developing a format for the proposal following known guidelines, identifying the objectives of the research project
and why anyone should care, discussing examples of successful proposal formats, developing a budget and cost assessment, interacting with program officers and agencies, and developing research partnerships.

3. Publishing Research Results in Peer Reviewed Journals

This workshop provides advice and training on publishing scientific and technical results in peerreviewed English language journals. Participants can bring an example of a paper or outline for an article they are considering for submission to a journal. Topics include publication and review process for many journals, organizing a paper, determining when and where to publish results, identifying data to include in the publication and organizing the material, and working with editors and on-line submissions and responding to reviews.

TIME TABLE

Time	Title / Facilitator
08:45- 09:00	Welcoming Remarks and Introduction of the Workshop
09:00- 10:30	Career Launch and Acceleration Pushpa Murthy
10:30 - 11:00	Coffee Break
11:00 - 12:30	Selling Your Science: The Art of Effective Proposal Writing Pushpa Murthy
12:30 - 14:00	Lunch Break
14:00 - 15:30	Publishing Research Results in Peer Reviewed Journals Abdelaziz El Jazouli
15:30 - 16:00	Concluding Remarks

Organizer: Priscilla Lewis
COACh Interim Co-Director
University of Oregon, USA
Email: cilla@uoregon.edu

11TH INTERNATIONAL CONFERENCE OF THE AFRICAN MATERIALS RESEARCH SOCIETY

" PRE-CONFERENCE WORKSHOPS "

Date: 10 -11 December 2022
Venue: University Cheikh Anta Diop of Dakar

VALUE CHAINS ENTREPRENEURSHIP FOR MATERIALS SCIENTISTS FROM AFRICA

FACILITATORS



Dr. Surya Raghu

ETCube International , U.S.A.
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Prof Balla Diop Ngom

Universite Cheikh Anta Diop de Dakar, Senegal
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BACKGROUND AND PURPOSE

A 2-day intensive workshop on Value Chain Innovation and Entrepreneurship will be organized during Dec. 10-11, 2022. Participants will be introduced to the basics concepts of value chains, and innovation and entrepreneurship in value chains specifically addressing opportunities for material scientists in coming up with innovative technical solutions to the needs of the industry and taking the ideas to the market by developing a viable business model, a sound business plan and a commercialization strategy.

GOALS AND TOPICS

The objectives of this Workshop are to introduce to the scientists the process of innovation, generation and protection of intellectual property, technology transfer and commercialization of inventions. The Workshop will consist of lectures by invited speakers, case studies, group discussions and role-playing sessions related to commercialization of a product.

Topics will include:

- Basics of value chains and importance of sustainable value chain resilience for industry
- Relation between scientific research, inventions and products with value chain planning

- Innovation/Research to market case studies
- Market need identification/feasibility study
- Concept of intellectual property (IP) and its significance in commercializing your ideas
- Business Model development
- Taking science to the market - Timelines and processes
- Doing business in Africa (components of the entrepreneurial ecosystem, business formalities, IP office, grants, investor resources, etc.)
- Finance – basic financial skills needed for start-ups
- Marketing and Sales
- Communication and networking skills
- Plenty of group exercises, networking and collaboration among participants
- Pitching your ideas to investors, customers, etc., business plan presentations by participants

Participation: About 50-participants (max) –Faculty, post-doc/postgrads, graduates/undergrads + a few observers
This program is for a selected and limited number of participants. It is particularly ideal for faculty-postdoc, faculty-post graduate/undergraduate students who are interested in learning innovation and entrepreneurial skills to commercialize their scientific inventions from their research. Participants from all branches of science, engineering and management related to material science are invited to apply for participation in the Workshop. Women candidates are strongly encouraged to apply. Selection of candidates will be based on their technical background to get a mix of disciplines and strong motivation to become innovators and entrepreneurs as evidenced in their application. Given the continuity of topics in the program, participants should be willing to attend all sessions on both days.

TIME TABLE

Day 1

Time	Session (tentative topics, to be finalized)
08:30 – 09:00	Welcome remarks and self-introductions, intro to workshop
09:00 -- 09:45	Intro to value chains, resilient value chains and sustainable value chains
09:45 -- 10:30	Identifying value chain niches in various industry from materials perspectives
10:30 – 11:00	Break
11:00 – 12:00	Generating business ideas based on value chain opportunities
12: 00 – 12:30	Feasibility analysis of business ideas
12:30 – 13:30	Lunch
13:30 – 14:30	Design thinking, Market Survey and evaluating customer feedback for your ideas value proposition – practicing a value proposition for your business ideas
14:30 – 15:30	Basics of Finance for entrepreneurs
15:30 – 16:00	Break
16:00 – 17:00	Introduction to Intellectual Property

Day 2

Time	Session (tentative topics, to be finalized)
08:30 – 09:30	Competition, Entry barrier and market analysis, price point, first customer, user feedback, endorsement, decision maker, etc.
09:30 -- 10:30	Business Models for start-ups
10:30 – 11:00	Break
11:00 – 12:30	Government incentives and sources of financing for start-ups in Senegal/Africa for Value Chain companies - 2 local speakers
12:30 – 13:30	Lunch
13:30 – 14:30	Estimating finances for a start-up and business plan development
14:30 – 15:30	How to pitch to an investor and investor expectations Pitching for cash: Equity issues, share dilution Understanding funding needs at different stages of a start-up Valuation at various stages of development. Presentation Skills
15:30 – 16:00	Break
16:00 – 17:00	Discussion and wrap-up

11TH INTERNATIONAL CONFERENCE OF THE AFRICAN MATERIALS RESEARCH SOCIETY

"PRE-CONFERENCE WORKSHOPS"

Date: 10 -11 December 2022
Venue: University Cheikh Anta Diop of Dakar

WORKSHOP ON PROPOSAL WRITING SKILLS FOR SCIENTIFIC USER FACILITIES

FACILITATORS



Dr. Zachary D. Hood
Argonne National Laboratory
USA
Email: zhood@anl.gov



Prof Abdou Lachgar
Wake Forest University,
USA
Email: lachgar@wfu.edu

WORKSHOP DESCRIPTION AND OBJECTIVE:

Proposals are critical in science; however, most if not all senior-level undergraduate and graduate-level courses overlook teaching practical skills in proposal writing. There is a very big difference between learning to write proposals and learning to write successful proposals. In this workshop, you will not only learn how to write an effective proposal for scientific user facilities, but more importantly learn how to write successful proposals. Participants in this workshop will develop proposal writing skills by preparing a 2-page proposal to access scientific user facilities. You will learn strategies to prepare proposals that detail an experiment (or series of experiments) to be performed at a Department of Energy (DOE) Scientific User Facility and/or a European User Facility. Many of these user facilities provide free access to complete high-level experiments and characterizations upon successful review of a proposal. In fact, some of these facilities may be of use to students during graduate studies.

This workshop will
1) expose participants to Scientific User Facilities in the United States and Europe,
2) teach participants how to write effective user proposals, and
3) show participants how user proposals are generally reviewed.

More specifically, participants will choose a User Facility and prepare a proposal

that describes one or more experiments that will advance our fundamental chemical and physical understanding of a specific material for a defined application. Prior to the workshop, participants will be provided readings on the most recent perspective and review articles from the following academic journals: Chemistry of Materials, Accounts of Chemical Research, Chemical Reviews, JMCA, JMCB, JMCC, Nature Materials, Nature Energy, and Nature Catalysis.

Sample topics include materials for the following applications:

- Biomaterials & Materials for Health
- Materials for Water & Environmental Monitoring
- Materials for Agriculture
- Materials for Energy
- Materials for Mining & Manufacturing
- Nanomaterials, Quantum Materials, Photonic Materials, & Nanotechnologies
- Computational Materials Science
- A topic of your choice

Participation: About 30-participants (max)
Audience: Undergraduate, Graduate, Postdoctoral/Postgraduate, Faculty Due to the interactive nature of this workshop, the organizers designed the program for a limited number of participants. This workshop is particularly ideal for undergraduate students, graduate students, postdoctoral/postgraduates, or faculty members who are interested in learning about Scientific User Facilities in the United States and Europe as well as the proposal writing and review process. Participants from all branches of science and engineering are invited to apply for participation in the Workshop. Women candidates are strongly encouraged to apply. Participants are expected to register at least two weeks before the workshop. They must choose a specific topic and complete 1) a GoogleForm, 2) a pre-proposal survey, and 3) suggested readings prior to the workshop. Participants are expected to attend all sessions on both days.

TIME TABLE

Workshop agenda (December 10, 2022):	
9:00 – 9:30	Introduction, review of pre-proposal survey, organization of material teams (3-4 participants per team)
9:30 – 10:00	Discussion with team members to decide on a specific topic
10:00 – 10:30	Share material with participants of the workshop
10:30 – 11:00	Coffee break
11:00–12:30	Interactive lecture on proposal writing and overview of the proposal writing canvas
12:30 – 14:00	Lunch break
14:00 – 16:00	Interactive session with the proposal writing canvas, research at scientific user facilities, and feedback to students
[Submit proposals by 12 pm local time on Dec. 11, 2022]	
Workshop agenda (December 11, 2022):	
13:00 – 14:00	Interactive peer review session
14:00 – 14:30	Share reviewer feedback
14:30 – 15:30	Preparation for group presentation
15:30 – 16:00	Coffee break
16:00 – 18:00	Presentation and defense of proposals (~10 minutes/team)
18:00 – 18:30	Certificate of completion

11TH INTERNATIONAL CONFERENCE OF THE AFRICAN MATERIALS RESEARCH SOCIETY

" PRE-CONFERENCE WORKSHOPS "

Date: 10 -11 December 2022
Venue: University Cheikh Anta Diop of Dakar

WORKSHOP ON SUSTAINABLE AND BIOMASS DERIVED MATERIALS FOR FUTURE ENERGY STORAGE

FACILITATOR



Prof. Ncholu Manyala

Pretoria, South Africa
E-mail: ncholu.manyala@up.ac.za

BACKGROUND AND PURPOSE

To equip participants with basic knowledge of electrochemical capacitors/Supercapacitors using nano-carbon derived from biomass and its composites with metal oxides/hydroxides to for hybrid supercapacitors. The expectation is that upon returning to their home institutions, the participants would be equipped with enough knowledge to make use of biomass wastes which are abandoned in Africa to convert them into useful materials as electrode materials for energy storage such as supercapacitors. The participants are also expected to be able to make a network within the AMRS which should lead to sustainable collaboration.

OUTLINE

Introduction of Electrochemical capacitors/Supercapacitors:
The Electrochemical capacitors/Supercapacitors are electrochemical energy storagedevices with high specific power, but moderate specific energy and bridge the gap between conventional capacitors with high power and batteries with high specific

energy. There three types of Electrochemical capacitors:
(i) Electric double layers capacitors (EDLC)
(ii) Pseudo-capacitors
(iii) Faradic capacitors or battery-type capacitors
These three types of supercapacitors will be discussed based on their mechanisms and relevant materials.

Electrolytes for Electrochemical capacitors:

There different types of electrolytes for supercapacitor which control the cell potential
of the device:
(i) Aqueous electrolytes
(ii) Organic electrolytes
(iii) Ionic liquids electrolytes

These electrolytes will be discussed to show the role they play in the electrochemical device.

Discussion on activated carbon from biomass wastes:

Activated carbon from biomass wastes as electrodes for electrochemical capacitors
Discussion will be based on the different sources of biomass wastes and synthesis methods of producing activated carbon. The use of such activated carbon as electrodes for electrochemical capacitors with specific examples. The symmetric devices as well as hybrid devices will be discussed.

TIME TABLE

Time	Activity
08:00 – 08:15	Introductions and the purpose of the workshop
08:15 – 10:00	Introduction of electrochemical capacitors and their properties
10:30 – 10:30	Break
10:30 – 12:30	Electrolytes and Activated carbon synthesis methods and characterization from biomass wastes
12:30 – 13:30	Lunch
13:30 – 15:30	Discussion of different examples of devices of AC from biomass
15:30 – 16:00	Beak
16:00 – 17:00	General discussion

11TH INTERNATIONAL CONFERENCE OF THE AFRICAN MATERIALS RESEARCH SOCIETY

" PRE-CONFERENCE WORKSHOPS "

Date: 10 -11 December 2022
Venue: University Cheikh Anta Diop of Dakar

PROMOTING ELECTROSPINNING IN AFRICA

FACILITATORS



Dr Samuel Chigome

Botswana Institute for Technology, Research and Innovation, Botswana
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Dr Ipe Mavunkal

Botswana Institute for Technology, Research and Innovation, Botswana
Email: imavunkal@bitri.co.bw

PURPOSE OF THE WORKSHOP;

To equip participants with the theoretical and experimental understanding of electrospinning. The expectation is that upon returning to their home institutions, the participants will be able to incorporate electrospinning in their research work with the goal of addressing Africa's challenges through collaborative work within the AMRS network and beyond.

OUTLINE

Introduction to electrospinning
Electrospinning is a technique that relies on repulsive electrostatic forces to draw a polymer solution
into nanofibers. The three most basic components of any electrospinning set-up are;
(i) Power supply
(ii) Source of a polymer solution
(iii) A collector
In order to control the electrospinning process, solution parameters, applied parameters and ambient parameters need to be optimized. The lectures will focus on teaching the participants the principle and experimental aspects of

needle, needleless and coaxial electrospinning at a laboratory scale.
Practical demonstration of laboratory scale electrospinning
The most basic electrospinning setup consists of the following;
(i) Pasteur pipette
(ii) Copper wire
(iii) Power supply
(iv) Aluminum foil and collecting stand
(v) Polymer solution

Building such a set-up to conduct experiments on nanofibers is affordable to any University in Africa. The practical demonstration will involve at least two set-ups, the most basic one and one in which a syringe pump, needle and syringe are use as polymer solution feed. 2.5 wt%, 5 wt%, 7.5 wt% and 10 wt% PEO (Mw 300 000) dissolved in water will be electrospun. Voltage, Distance and flow rate will be varied, and fibers collected for a maximum of a minute onto a glass slide. A light microscope and SEM will be used to obtain images.

PILOT SCALE AND INDUSTRIAL SCALE ELECTROSPINNING

The lectures will present the pilot scale facilities at BITRI and Industrial scale facilities that are on the market. Practical considerations for scaling up electrospinning will be presented.

PRACTICAL ASPECTS OF ELECTROSPUN FIBER PRODUCT DEVELOPMENT

The different ways of handling nanofiber membranes which may include heat treatment, or mechanical strength enhancement among other approaches with a specific product in mind will be presented. Examples of electrospun nanofiber-based products will be presented.

DISCUSSION ON ELECTROSPUN NANOFIBER-BASED SOLUTIONS FOR AFRICA

Participants will propose ideas on how they think electrospinning can be used to address Africa's challenges. It is expected that plans for setting up electrospinning facilities at their home institutions will be discussed and establishment of links for collaborative work within the AMRS network.

TIME TABLE

Time	Activity
0800-0830	Introductions and purpose of the workshop
0830-1000	Introduction to Electrospinning
1000-1030	Break
1030-1230	Practical demonstration of laboratory scale electrospinning
1230-1330	Lunch
1330-1430	Pilot scale and Industrial scale electrospinning
1430-1530	Practical aspects of electrospun fiber product development
1530-1600	Break
1600-1700	Discussion on electrospun nanofiber-based solutions for Africa

11TH INTERNATIONAL CONFERENCE OF THE AFRICAN MATERIALS RESEARCH SOCIETY

"PRE-CONFERENCE WORKSHOPS"

Date: 10 -11 December 2022
Venue: University Cheikh Anta Diop of Dakar

WORKSHOP ON BIOSENSORS: MEASURING GLUCOSE AND THE CLINICAL IMPACT OF ACCURACY.

FACILITATOR



Prof. Elizabeth Hall

University of Cambridge, United Kingdom
Email: eah16@cam.ac.uk

BACKGROUND AND PURPOSE

To equip participants with a basic knowledge of biosensors and the use of the glucose test-strip as an exemplar that is widely used. The participants will learn how a glucose biosensor works and will examine the data collected from glucose teststrips and calculate accuracy and precision using statistical data analysis. Based on the outcomes, we will consider what the clinical impact on the treatment might be on the patient, if the measurement isn't perfectly accurate or precise. The expectation is that upon returning to their home institutions, the participants will understand the principles of biosensors and be equipped to understand that the accuracy of a medical diagnostic can impact treatment given to a patient. The participants are also expected to be able to make a network within the AMRS which should lead to sustainable collaboration.

OUTLINE

Introduction to Biosensors:
A biosensor is a self-contained integrated analytical device (a diagnostic), which is capable of providing specific quantitative or semi-quantitative analytical information using a biological recognition element (biochemical receptor) which is retained in direct spatial contact with an transduction element. A most important component of a Biosensor is the biological

recognition elementt that is used to:

(i) recognize the analyte
(ii) generate a signal that can be measured, directly or through a labeling or mediation system Biosensors have mainly been developed for medical diagnosis and management of health and were especially highlighted in the Covid 19 pandemic with the lateral flow assays. However, the first biosensor which used amperometric electrochemistry measured glucose. The history of amperometric biosensors is linked with that of blood glucose monitoring.

THE GLUCOSE BIOSENSOR:

Blood glucose monitoring plays a crucial role in the management of diabetes. Glucose biosensors provide real-time information on the changes in glucose concentration. The glucose biosensor technology helps individuals maintain normal blood glucose levels.
The rising prevalence of diabetes worldwide, technological advancements in selfmonitoring of blood glucose, and growing awareness about point on care (POC) testing are the key factors boosting demand for glucose monitoring biosensors. The increasing number of people suffering from diabetes among the urban population is boosting the demand for glucose monitoring biosensors.

Amperometric glucose biosensors have been divided into three generations. The first-generation biosensors were proposed by Clark and Lyons and became called enzyme electrodes. We will discuss the 3 generations of glucose biosensors and look at some examples of these biosensors that are in use today. Discussion on accuracy and precision and the development of an error grid for glucose determination:
We can see differences between the actual glucose concentration and the measured glucose concentration, so how we can understand the differences, and does it matter? We will look at how the data are affected by accuracy and precision and we will discuss the statistical methods we need to use to give us information for comparing devices and seeing how a device performs and how the data are distributed. We will then learn about Error Grid Analysis (EGAs) and how the development of EGAs for glucose measurement provide guidance on the impact of measurement error on clinical intervention.

TIME TABLE

Time	Activity
08:00 – 08:15	Introductions and the purpose of the workshop
08:15 – 10:00	Introduction to Biosensors and the Glucose Biosensor
10:30 – 10:30	Break
10:30 – 12:30	Using a Glucose Biosensor
12:30 – 13:30	Lunch
13:30 – 15:30	Analysing data from the Glucose Biosensor and its clinical impact
15:30 – 16:00	Break
16:00 – 17:00	General discussion

11TH INTERNATIONAL CONFERENCE OF THE AFRICAN MATERIALS RESEARCH SOCIETY

"PRE-CONFERENCE WORKSHOPS"

Date: 10 -11 December 2022
Venue: University Cheikh Anta Diop of Dakar

WORKSHOP ON LIFE CYCLE ASSESSMENT

FACILITATORS



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PURPOSE OF THE WORKSHOP

Globally, decisions being made by government leaders, business executives, and those in academia are becoming more data-driven. This includes pressing decisions regarding our ability to sustain, and hopefully thrive, as a society. One technique used broadly to inform these decisions is life cycle assessment (LCA). LCA is a tool that is used to quantify the environmental, economic, and social impacts of all life cycles (production, consumption, disposal) of a particular product, process, or service. All inputs and outputs of the process are accounted for and an overall idea of the relative sustainability of the system is created. LCA can be applied broadly and has resulted in significant policy decisions worldwide.

This workshop aims to educate participants on the principles and application of LCA and teach the initial steps in planning and executing their own impactful LCA. It is geared to be hands-on with participants actively taking part in the discussion of LCA case studies. A free online learning course on LCA provided by the University of Michigan Center for Socially Engaged Design (CSED) will be introduced for continuing education after the workshop. Furthermore, there will be an opportunity for participants in the workshop to apply for free access to state of the art LCA modelling software as well as support in ideating and executing their own LCAs. In addition, an introduction to techno-economic assessment (TEA) will be provided.

OUTLINE

- Sustainability is about People: How can LCAs be used to drive change?
- Introductory example of how people drive environmental change now and for future generations

- Introduction to the workshop and teaching methods that will be used (think, pair, share methodology)
- Case Study on Challenging Sustainability: How "green" are electric motorcycles?
- Conversation on the electrification of motorcycles in East Africa with potential benefits and drawbacks environmentally, economically, and socially
- Four Criteria Interactive Activity
- What are the four criteria for a sustainable system? How do we apply them?
- Several examples are evaluated for passing/failing the criteria using the think/pair/share paradigm to facilitate discussion
- What happens when you don't use an LCA? Selecting a meaningful comparison.
- What is LCA useful for? What is it not useful for? Myths and misunderstandings around LCA
- Setting the goal and scope of a study, creating a life cycle inventory of data for analysis, selecting an impact assessment methodology that is relevant to the study, and conducting a sensitivity analysis
- Case Study: Biologically-grown Cement for Sustainable Construction
- Learning the components of the LCA through in-depth through discussion of a sustainable building material alternative
- Interactive Activity on Setting a Goal and Scope
- Several energy and material systems will be discussed by participants and the first step of setting up an LCA, figuring out the Goal and Scope, will be facilitated.
- Live Demo of Modelling Software/Tips for conducting a complete LCA
- The JUAMI Open Computing Facility and Umberto LCA modelling software will be demoed
- Pointers will be provided on completing the next steps in the process, presenting your results in an impactful way, and providing recommendations
- Overview of LCA Resources Available and Closing Remarks
- Online course on LCA through U. of Michigan, application for access to LCA software, support on ideating and executing an LCA

TIME TABLE

Time	Activity
0800-0820	People-focused Sustainability: How can LCAs be used to drive change?
0820-0845	Challenging Sustainability: Electrification of Motorcycles in East Africa
0845-0850	Break
0850-0930	Four Criteria Interactive Activity
0930-1000	What is an LCA/Making a Meaningful Comparison Using LCA
1000-1020	Break
1020-1030	Recap LCA information (Goal and Scope, Inventory, Impact Assessment)
1030-1130	Case Study: Biologically-grown Cement for Sustainable Construction
1130-1140	Break
1140-1230	Interactive Activity on Setting up an LCA
1230-1245	Live Demo and Tips
1245-1315	Introduction to Techno-economic analysis
1315-1345	Overview of LCA Resources Available and Closing Remarks



AMRS2022
MAIN CONFERENCE

PROGRAMME

Day-1 12-12-2022		
08.00-09.00	**Registration**	
09.00-10.15	Welcome Address: Prof Aboubaker Chedikh Beye, AMRS, Doyen FST, Recteur UCAD, MESRI, Presidence Plenary Talk-00: Safety on site and Destination Senegal	Press/ Media
10.15-10.30	Plenary Talk-01: Prof Geraldine Richmond	Prof Mohamed CHAKER
10.30-11.30	Plenary Talk-02: Nobel Laureat Prof Gerard Mourou	
11.30-12.00	**Tea Break**	
12.00-12.30	Plenary Takl-03**:** DI-01: Prof Malik Maaza	Dr Samuel CHIGOME
12.30-13.00	Plenary Talk-04: DI-02: Prof Wole Soboyejo	
13.00-13.30	Plenary Talk-05: GI-01: Prof Magdalena Titirici	
13.30-14.30	**Lunch Break**	
14.30-15.50	Keynotes Panel: Materials for Agriculture - *Prof A. T. DIOP, Université Amadou Makhtar MBOW, Senegal* - *Dr C. Dimkpa, Connecticut Agricultural Experiment Stations, USA/Nigeria* - *Dr S. Santra, University of Central Florida, USA/India* Panel Discussions:	Prof DIAGA DIOUF & Dr ABDOULAYE THIAM
15.50-17.10	Keynotes Panel: Materials for Water and Environment Monitoring - *Prof. M. Thuo, Iowa State University, USA* - *Prof S. Garcia-Segura, Arizona State University, USA* - *Prof. E. Moretti, Ca' Foscari University of Venice, Italy* Panel Discussions	
17.10-17.25	**Tea Break**	

Day-1 12-12-2022								
	Talks in Parallel Symposium (Invited, EC: Early Careers and OP: Oral Presentation)							
17.30-18.30	**S1:** Materials for Construction, Mining and Manufacturing	**S2 & *S8*** *Materials for Agriculture & Education and Networking in Materials Science & Engineering*	**S3:** Materials for Energy	**S4:** Materials for Water & Environment	**S5:** Biomaterials and Materials for Health	**S6:** Nanomaterials, Quantum Materials, Photonics Materials & Nanotechnologies	**S7:** Computational Materials	**Sides Events**
Invited SESSION 17.30-18.30	**Moderator: Prof PETER A. OLUBAMBI**	**Moderator: Prof CHRISTIAN DIMPKA**	**Moderator: Prof Ncholu Manyala**	**Moderator Prof MOHAMED SIAJ**	**Moderator: Prof SERGIO E. MOYA**	**Moderator: Prof FIORENZO VETRONE**	**Moderator: Prof HASANI CHAUKE**	**Sides Events**
17.30-17.50	Invited-1 Prof SAID KENAI	Invited-1 Prof DIAGA DIOUF	Invited-1 Prof FRANCESCO ROSSELLA	Invited-1 Prof ABDULKAREEM AMBALI SAKA	Invited-1 Prof. JOHAN FOSTER	Invited-1 Prof. CHRISTIANA A NIJHUIS	Invited-1 Dr ALLE DIOUM	
17.50-18.10	Invited-2 Prof ADAMS TIDJIANI	Invited-2 Prof NICOLAS MUECKE	Invited-2 Prof DIOUMA KOBOR	Invited-2 Prof. SABELO D. MHLANGA	Invited-2 Prof. ELIZABETH (LISA) HALL	Invited-2 Prof ALIAN DUFRESNE	Invited-2 Prof. NELSON Y. DZADE	
18.10-18.30	Invited-3 Dr KOLAWOLE ADISA OLONADE	Invited-3 Dr ISSA FAYE	Invited-3 Prof PIERRE KALENGA MUBIAYI	Invited-3 Dr MANOKO MAUBANE-NKADIMENG	Invited-3 Prof FEDERICO POLO	Invited-3 Prof ALBERTO VOMIERO	Invited-3 Prof KULBIR GHUMAN	
18.30…	**End of Day-1**							

Day-2 13-12-2022								
08.00-09.00	**Registration**							
09.00-09.30	Plenary Talk-06: GI-02: *Prof Malika Jeffries-EL* **Moderator Prof. Magdalena TITIRICI**							
09.30-10.50	Keynotes Panel: Photonics - *Prof Souleymane O Diallo* - *Dr Moussa N'gom* - *Dr Abdoulaye Ndao* Panel Discussions **Moderator: Prof MARK W. HORN**							
10.50-11.00	**Tea Break**							
11.00-13.30	Talks in Parallel Symposium (Invited, EC: Early Careers and OP: Oral Presentation)							
	S1 Materials for Construction, Mining and Manufacturing	S2 & S8 *Materials for Agriculture & Education and Networking in Materials Science & Engineering*	S3 Materials for Energy	S4 Materials for Water & Environment	S5 Biomaterials and Materials for Health	S6 Nanomaterials, Quantum Materials, Photonics Materials & Nanotechnologies	S7 Computational Materials	S9 Special focus session on cement and concrete Side event by PTB/BAM - PUBLIC -
Invited SESSION 11.00-11.40	**Moderator Dr KATRINA RAMIREZ-MEYERS**	**Moderator Dr ALASSANE TRAORE**	**Moderator Dr CLARA SANTATO**	**Moderator Dr MANOKO MAUBANE-NKADIMENG**	**Moderator Prof JOHAN FOSTER**	**Moderator Prof CHRISTIANA A NIJHUIS**	**Moderator Prof. NELSON Y. DZADE**	**Moderator Dr. Wolfram Schmidt Intro by PTB/BAM**
11.00-11.20	Invited-04 Prof PETER A. OLUBAMBI	Invited-04 Dr IFRIKY TADADJEU	Invited-04 Dr ZACHARY D. HOOD	Invited-04 PROF KOVO ABDULSALAMI SANNI	Invited-04 Prof LUAI R. KHOURY	Invited-04 Prof FIORENZO VETRONE	Invited-04 Prof HASANI CHAUKE	Natural pozzolana Mr. NABIL BELLA
11.20-11.40	Invited-05 Dr TAKALANI MADZIVHANDILA	Invited-05 Prof OSSEO-ASARE KWADWO ASARE	Invited-05 Prof GIOVANNI FANCHINI	Invited-05 Dr ELIZABETH N. NDUNDA	Invited-05 Prof SERGIO E. MOYA	Invited-05 Prof JEROME P. CLAVERIE	Invited-05 Prof SERIGNE BIRA GUEYE	Laterite binders Dr. ELIE KAMSEU

Day-2 13-12-2022								
OP SESSION 11.40-13.30	**Moderator Dr PHILBERT NSHIMIYIMANA**	**Moderator Dr ALASSANE TRAORE**	**Moderator Prof PIERRE KALENGA MUBIAYI**	**Moderator Prof. SABELO D. MHLANGA**	**Moderator Prof LUCIEN WEISS**	**Moderator Dr SIDIKI ZONGO**	**Moderator Dr JEAN PAUL LATYR FAYE**	**Moderator Prof. MARTIN PALOU**
11.40-11.55	OP-01 MOULOUD ABDESSEMED	OP-01 MOHAMED NAJIB SECK	OP-01 BENJAMIN AGYEI-TUFFOUR	OP-01 SIYABONGA A. MHLONGO	OP-01 ANELISIWE MBENGASHE	OP-01 BOITUMELO MAKGABUTLANE	OP-01 VICTOR ODARI	Chemcial admixtures Dr. Dipl.-Ing. WOLFRAM SCHMIDT
11.55-12.10	OP-02 PAUL M. LEKOADI	OP-02 DHANUSH UDAYASHANKARA JAMADGNI	OP-02 BAYE MODOU NDIAYE	OP-02 NOOR JEHAN GULAMUSSEN	OP-02 ROLIVHUWA BISHOP RAMAGOMA	OP-02 SEBASTIAN WAITA	OP-02 ROBINSON MUSEMBI	Cement analysis Prof. KAREN SCRIVENER
12.10-12.25	OP-03 DESIRE M.K. ABRO	OP-03 SIMEON DIEDHIOU	OP-03 ESTHER OBONYO	OP-03 AFONSO DANIEL MACHECA	OP-03 KIYAASHA DYAL UKABHAI	OP-03 DIALLO ABDOUL KADRI	OP-03 ABASS AKANDE FAREMI	Case study Algeria Prof. SAID KENAI
12.25-12.40	OP-04 SAMUEL SKHOSANE	OP-04 DESMOND. E.P KLENAM	OP-04 JUVET. N. FRU	OP-04 AGNES PHOLOSI	OP-04 MARTIN ONANI	OP-04 TOMI K. BAIKIE	OP-04 BONGANI NGOBE	Case Study Ghana Dr Mark Bediako
12.40-12.55	OP-05 FAREED DAWAN	OP-05 MICHAEL OLUWATOSIN BODUNRIN	OP-05 BINET BOUESSO	OP-05 BALLA FALL	OP-05 TUNDE VICTOR OJUMU	OP-05 BONAKELE P. MTOLO	OP-05 RAMOGOHLO DIALE	Case study Kenya Prof. SYLVESTER ABUODHA
12.55-13.10	OP-06 AKINDEHINDE AYOTUNDE AKINDAHUNSI	OP-06 MUHAMMAD ABDULLAH	OP-06 SIZWE B SIBIYA	OP-06 MAZIYA KHONA	OP-06 EL HADJI DIENG	OP-06 ABDOULAYE DIALLO	OP-06 TEBOGO LEDWABA	Statistics and results of the 4rth pan-African Cement Proficiency Scheme PACE-PTS Dr. WOLFRAM SCHMIDT and Ms. PHELADI TLHATLHA
13.10-13.25	OP-07 YOUNOUSSA MILLOGO	-	OP-07 BOKOME SHAKU	OP-07 JANUARIO DA COSTA HOSSI	OP-07 DURVA ARUN NAIK	OP-07 KGOMOTSO N.G. MTSHATSHENI	OP-07 ALLE DIOUM	

Day-2 13-12-2022		
13.25-14.30	**Health Break: Lunch**	
14.30-15.50	Keynotes Panel: Nanomaterials, Quantum Materials, Photonics Materials & Nanotechnologie - *Prof H. Winful, University of Michigan, USA* - *Prof M. Diale, University of Pretoria, South Africa,* - *Prof M. Henini, University of Nottingham, UK* Panel Discussions: **Moderator Dr MOUSSSA NGOM**	**Internal PTB workshop: - not public - Results discussions of the pan-African Cement Testing Round Robin**
15.50-17.10	Keynotes Panel: Biomaterials and Materials for Health - *Prof. P. S. Weiss, University of California, Los Angeles, USA* - *Prof M. Sosnik, Technion-Israel Institute of Technology, Israel* - *Prof T. H.R. Niepa, University of Pittsburgh, United States* Panel Discussions: **Moderator Prof. NICHOLAS A KOTOV**	
17.10-19.00	**Tea Break & Posters Session**	
19.00	**End of the Day**	

Day-3 14-12-2022								
08.00-09.00	**Registration**							
09.00-09.30	Plenary Talk-07: GI-03 Prof Sossina Haile **Moderator: Prof M. DIALE**							
09.30-10.50	Keynotes Panel: Materials for Construction, Mining and Manufacturing - *Prof L. Cornish, WITS, South Africa* - *Dr W. Schmidt, BAM, Germany* - *Dr K. Scrivener,* Panel Discussions: **Moderator Prof SAID KENAI**							
10.50-11.05	**Tea Break**							
11.05-13.45	Talks in Parallel Symposium (Invited, EC: Early Careers and OP: Oral Presentation)							
	S1 Materials for Construction, Mining and Manufacturing	S2 & *S8* *Materials for Agriculture &* *Education and Networking in Materials Science & Engineering*	**S3** Materials for Energy	**S4** Materials for Water & Environment	**S5** Biomaterials and Materials for Health	**S6** Nanomaterials, Quantum Materials, Photonics Materials & Nanotechnologies	**S7** Computational Materials	**S9** Special focus session on cement and concrete Side event by PTB/BAM- PUBLIC -
Invited SESSION 11.05-11.45	**Moderator Dr TAKALANI MADZIVHANDILA**	**Moderator MUHAMMAD ABDULLAH**	**Moderator Dr BENJAMIN AGYEI-TUFFOUR**	**Moderator PROF KOVO ABDULSALAMI SANNI**	**Moderator Dr ROLIVHUWA BISHOP RAMAGOMA**	**Moderator Prof FABIAN EZEMA**	**Moderator Prof ROBINSON MUSEMBI**	**Moderator Prof KOLAWOLE OLONADE**
11.05-11.25	Invited-06 Dr KATRINA RAMIREZ-MEYERS	Invited-06 Dr ALASSANE TRAORE	Invited-06 Prof DAVID DODOO-ARHIN	Invited-06 Dr BENTON OTIENO	Invited-06 Prof LUCIEN WEISS	Invited-06 Prof NICOLA PINNA	Invited-06 Prof OMOLOLU AKIN-OJO	Chloride resistance Dr. AKINDEHINDE AYOTUNDE AKINDAHUNSI
11.25-11.45	Invited-07 Dr INES NGASSAM	Invited-07 Dr MATAR SYLLA	Invited-07 Prof PATRICK SHARROCK	Invited-07 Prof MOHAMED SIAJ	Invited-07 Prof. FRANCESCO STELLACCI	Invited-07 Prof MARK W. HORN	Invited-07 Prof ADJI BOUSSO DIENG	Alkali-aggregate reaction JANINA KANJEE

Day-3 14-12-2022								
OP SESSION 11.45-13.30	**Moderator Dr FARAI CHRISPEN BANGANAYI**	**Moderator MUHAMMAD ABDULLAH**	**Moderator Dr CECIL K. KING'ONDU**	**Moderator Dr ELIZABETH N. NDUNDA**	**Moderator Dr MALUTA STEVEN MUFAMADI**	**MODERATOR Dr ABDOULAYE DIALLO**	**Moderator Dr VICTOR ODARI**	**Moderator JANINA KANJEE**
11.45-12.00	OP-8 BEN FESTUS	Invited-08 Dr KIMBERLY SCOTT	OP-08 TOMI K. BAIKIE	OP-08 NAFISSATOU IDRISSA	OP-08 PATRICK MENSAH	OP-08 SALIF SOW	OP-08 MAHAMAT BICHARA ABDERAMAN	Lightweight aggregates Dr. JULIA SEHER
12.00-12.15	OP-9 BAYE OUMAR DIOP		OP-09 MIRIAM ABADE-ABUGRE	OP-09 KGOMOTSO N.G. MTSHATSHENI	OP-09 YIPORO DANYUO	OP-09 ALANA PAULS	OP-09 RAZIEH MORAD	Iron rods Ms. ADELAIDE AIKINS
12.15-12.30	OP-10 YAWO DANIEL ADUFU	-	OP-10 VLADIMIR KHOVAYLO	OP-10 JIMOH OLADEJO TIJANI	OP-10 JOEY CHIFAMBA	OP-10 WALY DIALLO	OP-10 MAHMOOD AKBARI	Climate adaption Dr. KOLAWOLE OLONADE
12.30-12.45	OP-11 NDEYE MAGATTE FALL	-	OP-11 N. MATINISE	OP-11 MAME NINY SENGHOR	OP-11 MPHO PHEHELLO NGOEPE	OP-11 BRIAN IEZZI	OP-11 KATELYN JONES	Environmental aspects Ms. PHELADI TLHATLHA
12.45-13.00	OP-12 AÏDA GAYE	-	OP-12 GLORIA IFUNANYA NGENE	OP-12 VERA BORDAH	OP-12 IPE MAVUNNKAL	OP-12 BM. MABAKACHABA	OP-12 DAVID MACHIRI	Decarbonisation Prof. MARTIN PALOU

Day-3 14-12-2022								
13.00-13.15	OP-13 MENADI BELKACEM	-	OP-13 SAEED SAEED	OP-13 JOHN MOMA	Invited-08 Prof JEAN F. FELLER	OP-13 NANDIPHA L. BOTHA	OP-13 MOUSTAPHA CAMARA	Internal PTB workshop: - Open - Challenges in testing cement in Africa
13.15-13.30	OP-14 JANINA KANJEE	-	OP-14 JESSE J. HINRICHER	OP-14 ADAMA D NGOM		OP-14 NIYONKURU DIEUDONNE	OP-14 KOLAWOLE K SHOLA	
13.35-14.30	**Health Break: Lunch**							
14.30-15.50	Keynotes Panel: Computational Materials Sciences - *Prof D. Bagayoko, Southern University, Baton Rouge, USA* - *Prof G-M Rignanese, UC Louvain, Belgium* - *Prof I. Dabo, Penn State, USA* Panel Discussions: **Moderator Prof S BIRA GUEYE**							Internal PTB workshop: - Open - Challenges in testing cement in Africa
15.50-17.10	Keynotes Panel: Materials for Energy - *Prof L. Vayssieres, Xi'an Jiaotong University, China* - *Prof F. ROSEI, INRS, Canada* - *Prof A. Djire, Texas A&M University, USA* Panel Discussions **Moderator: Prof NCHOLU MANYALA**							
17.10-17.30	**Health Break**							

Day-3 14-12-2022					
17.30-19.00	**EARLY CARERS PANEL SESSION: Focus on Early-Career Development—Insights from African Academia and Industry and African Scientifics Diaspora**				
	S1 Materials for Construction, Mining and Manufacturing	**S3** Materials for Energy	**S4** Materials for Water & Environment	**S6** Nanomaterials, Quantum Materials, Photonics Materials & Nanotechnologies	**S7** Computational Materials
17.30-19.00	**Dr KHADIM NDIAYE** Université Cergy Pontoise, France **Dr Walid YAHIAOUI** University of Blida 1, Algeria **PHILBERT NSHIMIYIMANA** University of Rwanda, Rwanda **Moderator:** Prof L. Cornish, WITS, South Africa	**Dr NDEYE F. SYLLA** University Cheikh Anta Diop, Senegal **Dr GEORGE BEPETE** Penn State University, USA/Zimbabwean **Dr KATLEGO MAKGOPA** Tshwane University of Technology, South Africa **Moderator:** Prof A. Djire, Texas A&M University, USA	**Dr BRIDGET K. MUTUMA** Kirinyaga University, Kenya **Dr ABDOULAYE THIAM** Universidad Tecnológica Metropolitana, Chili **EL HADJI MAMOUR SAKHO** University Cheikh Anta Diop, Senegal **Moderator:** Prof. Elisa Moretti, Ca' Foscari University of Venice, Italy	**Dr IBRAHIMA NGOM** University Cheikh Anta Diop, Senegql **Dr SIDIKI ZONGO** Université joseph kizerbo Burkina Faso **Dr FORCE T. THEMA** Botswana University of Agriculture & Natural Sciences, Botswana **Dr I. G. MADIBA** **iThemba LABS-NRF** **South Africa** **Moderator:** Prof M. Diale, University of Pretoria, South Africa,	**Dr CAROLINE R. KWAWU** Kwame Nkrumah University of Science and Technology, Ghana **Dr MAKHA NDAO** Université Amadou Mahtar MBOW, Senegal **Dr CHEIKH T. BOP** CNRS-Université Le Havre Normandie, France **Dr JEAN P. LATYR FAYE** University Cheikh Anta Diop of Dakar, Senegal **Moderator:** Prof D. Bagayoko, Southern University, Baton Rouge, USA
19.00	**End of Day-3**				

Day-4 15-12-2022							
08.00-09.00	**Registration**						
09.00-09.30	Plenary Talk-06: *Dr. MAMADOU DIALLO* **Moderator: Prof FABIAN I. EZEMA**						**SIDE EVENT Internal PTB workshop: - non-public - Standardisation challenges and specific African requirements**
9.30-10.50	Keynotes Panel: *Education and Networking in Materials Science & Engineering* - *Prof M. L. SAGNA, WPI, USA* - *Dr S. Rahgu, Ectube, USA* - *Prof M. M. Faye, UCAD, Senegal* Panel Discussions: **Moderator Dr SAMUEL CHIGOME**						
10.50-11.10	**Tea Break**						
	Talks in Parallel Symposium (Invited, EC: Early Careers and OP: Oral Presentation)						
	S1: Materials for Construction, Mining and Manufacturing	S3: Materials for Energy	S4: Materials for Water & Environment	S5: Biomaterials and Materials for Health	S6: Nanomaterials, Quantum Materials, Photonics Materials & Nanotechnologies	S7: Computational Materials	**SIDE EVENT Internal PTB workshop: - non-public - Standardisation challenges and specific African requirements**
Invited SESSION 11.10-11.30	**Moderator Dr INES NGASSAM**	**Moderator Dr GEORGE BEPETE**	**Moderator Dr EL HADJI MAMOUR SAKHO**	**Moderator Prof. FRANCESCO STELLACCI**	**Moderator Dr IMANE ADRAOUI**	**Moderator Dr MAHMOOD AKBARI**	
Day-4 15-12-2022							

11.10-11.30	Invited-8 Dr FARAI CHRISPEN BANGANAYI	Invited-8 Dr CLARA SANTATO	Invited-8 Prof THOKOZANI XABA	Invited-9 Prof. NICHOLAS A KOTOV	Invited-8 Prof FABIAN EZEMA	Invited-8 Prof KHOMOTSO P MAENETJA	**SIDE EVENT** **Internal PTB workshop:** **- non-public -** **Way forward Future specifications**
OP SESSION *11.30-13.15*	**Moderator**	**Moderator Dr KATLEGO MAKGOPA**	**Moderator Dr BRIDGET K. MUTUMA**	**Moderator Prof. FRANCESCO STELLACCI**	**Moderator Dr IBRAHIMA NGOM**	**Moderator Dr MAHMOOD AKBARI**	
11.30-11.45	-	OP-15 SARAT ALABIDUN	OP-15 BRENDA VOUNKI	Invited-10 Prof MOUHAMADOU HABIB SY	OP-15 CHEIKH BIRAHIM NDAO	OP-15 G. DIMITRI NGANTSO	
11.45-12.00	-	OP-16 MENGNAN WANG	OP-16 ADEWALE O. ADELOYE		OP-16 ALIOUNE AIDARA DIOUF	OP-16 BIMBADI S. G. ETUCHE	
12.00-12.15	-	OP-17 Dr CECIL K. KING'ONDU	OP-17 MARY SIMIYU TAABU	Invited-11 Dr MALUTA STEVEN MUFAMADI	OP-17 EL HADJI OUMAR GUEYE	OP-17 ATOUMANE NDIAYE	
12.15-12.30	-	OP-18 FRANCIS AKO MARLEY	OP-18 THAPELO MANYEPEDZA		OP-18 INNOCENT NKURIKIYIMFURA	-	
12.30-12.45	-	OP-19 LAT GRAND NDIAYE	OP-19 ABDOU KARIM DIALLO	Invited-12 Prof PAPA BIRAME GNING	OP-19 IMANE ADRAOUI	-	
12.45-13.00	-	OP-20 MODOU DIOP	OP-20 BEN BAKER		OP-20 SYLVESTER.M. MBAM	-	
13.00-13.15	-	OP-21 VUSANI M. MAPHIRI	OP-21 SELASSIE GBOGBO	Invited-13 HAYOUNI EL AKREM	OP-21 HAVLIK MIKA MARTIN	-	
13.15-14.30	**Lunch Break**						
14.30-16.00	**Closing Remarks……**						
16.00-19.00	**Excursion : Gorée, Monument de la Renaissance, Pink Lake, etc.**						
19.00-02.00	**Gala Diner**						

Gala Diner Program : 15-12-2022							
20.00	Openning						
20.30 - 21.30	Animation						
21.00 - 22.30	Feedback from Parallel Symposium and Prizes for Best orals and Posters presentations						
	S1: Materials for Construction, Mining and Manufacturing	S2 : *Materials for Agriculture*	S3 : Materials for Energy	S4: Materials for Water & Environment	S5: Biomaterials and Materials for Health	S6: Nanomaterials, Quantum Materials, Photonics Materials & Nanotechnologies	S7 : Computational Materials
22.30 - 00.00	Closing Remarks and Vote of Thanks						
00.00 - 02.00	Party						
02.00 - End	End of the AMRS conference						



PLENARY SPEAKERS

11TH INTERNATIONAL CONFERENCE OF THE AFRICAN MATERIALS RESEARCH SOCIETY

Date: 12-15 December 2022
Venue: University Cheikh Anta Diop of Dakar

PLENARY SPEAKER



Geraldine (Geri) Richmond
Department of Energy,
USA
Email: geraldine.richmond@hq.doe.gov

Dr. Richmond oversees the U.S. Department of Energy's Office of Science, the largest federal sponsor of basic research in the physical sciences in the U.S., DOE's applied R&D offices of Energy Efficiency and Renewable Energy, Fossil Energy and Carbon Management, Nuclear Energy, and Electricity as well as 13 of DOE's national laboratories.

She is on leave from the University of Oregon where she holds the Presidential Chair in Science and Professor of Chemistry. Her research focuses on laser-based and computational methods to understand the structure and dynamics at liquid surfaces with relevance to environmental and technological interests. She is a member of the U.S. National Academy of Sciences and has received numerous awards including the National Medal of Science.

11TH INTERNATIONAL CONFERENCE OF THE AFRICAN MATERIALS RESEARCH SOCIETY

Date: 12-15 December 2022
Venue: University Cheikh Anta Diop of Dakar

PLENARY SPEAKER



Prof Gérard Mourou

Nobel Laureate in Physics 2018

Gérard Mourou is Professor Haut-Collège at the École polytechnique. He is also the A.D. Moore Distinguished University Emeritus Professor of the University of Michigan. He received his undergraduate education at the University of Grenoble (1967) and his Ph.D. from University Paris VI in 1973.

He has made numerous contributions to the field of ultrafast lasers, high-speed electronics, and medicine. But, his most important invention, demonstrated with his student Donna Strickland while at the University of Rochester (N.Y.), is the laser amplification technique known as Chirped Pulse Amplification (CPA), universally used today. CPA revolutionized the field of optics, opening new branches like attosecond pulse generation, Nonlinear QED, compact particle accelerators. It extended the field of optics to nuclear and particle physics. In 2005, Prof. Mourou proposed a new infrastructure ; the Extreme Light Infrastructure (ELI), which is distributed over three pillars located in Czech Republic, Romania, and Hungary. Prof. Mourou also pioneered the field of femtosecond ophthalmology that relies on a CPA femtosecond laser for precise myopia corrections and corneal transplants.

Over a million such procedures are now performed annually. Prof. Mourou is member of the U.S. National Academy of Engineering, and a foreign member of the Russian Science Academy, the Austrian Sciences Academy, and the Lombardy Academy for Sciences and Letters. He is Chevalier de la Légion d'honneur and was awarded the 2018 Nobel Prize in Physics with his former student Donna Strickland.

11TH INTERNATIONAL CONFERENCE OF THE AFRICAN MATERIALS RESEARCH SOCIETY

Date: 12-15 December 2022
Venue: University Cheikh Anta Diop of Dakar

PLENARY SPEAKER



Prof. Aboubaker Chédikh BEYE

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Professor Aboubaker Chédikh BEYE is a distinguished and an EMERITUS from the Université Cheick Anta Diop of Dakar (UCAD). Vice President of RESSCO, Réseau de Compétences, Sénégal. Professor BEYE is an International Expert-Consultant (UNDP, IEPF francophonie, UN-GEF, UN-ILO, CRERE/CEDEAO).

Professor Aboubaker Chédikh BEYE earned a Doctorate (3rd Cycle) degree in Solid state from the university of Montpelier in 1980 and a Ph.D in 1987 Physics/Energy from the University of Nice/Sophia-Antipolis, France. He joined the Université Cheikh Anta DIOP de Dakar (UCAD) as Assistant Professor at the Department of Physics (Faculty of Sciences and Technologies) from 1980 to 1983 before being promoted to full Professor.

Acting for several years as a Principal Member of Technical Staff and research Director at the Laboratory of Physics and Applications, Prof BEYE, hold several positions. From 2018 to 2019, he was appointed as the Manager of the Institutional Support Project funded by the African Development Bank (ADB) for the African Peer Review Mechanism (APRM). In 2017 he was Director of Graduate School of Sciences-Technologies-Health and Environment at UCAD, while being a Senior Scientific Adviser, CRGM, Ministry of Mines and Geology in Brazzaville, Congo. From 2005 to 2016 Prof BEYE led as Director of the African Institute for Mathematical Sciences Mbour (Senegal). In addition, he was nominated Full Professor in Innovation Technology, TIC Incubator and Renewable Energy Incubator at the Université de Bambey, Sénégal. Also, from 2005-2007, Prof BEYE is appointed as CEO of The African Laser Centre in Pretoria, South-Africa. In the 90th, He has been twice invited as visiting scientist in Japan. Besides the abovementioned, Prof BEYE hold positions that also include Chairman of NANOAFNET, General Secretary and Board member of the African Material Research Society (AMRS). He has been bestowed with a number of national and international awards that include the Prix Re-source SUNUNET 2017 for his scientific contribution. He has been honored as International Scientist of the Year 2007 in Nanophotonics and Material Science by the International Biographical Centre of the University of Cambridge.

From his contribution to the field of science, He has authored and Co-authored more than 200 international peer reviewed ISICSI publications in reputable journals. From the education and the human capital development perspective, Prof. BEYE has attracted and trained a significant cohort of postgraduate students (more than 100 MSc and PhD students).

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PLENARY SPEAKER



Prof Wole Soboyejo

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Wole Soboyejo received a BSc in mechanical engineering from King's College London in 1985, and a PhD in materials science and metallurgy from Cambridge University in 1988. He worked as a Research Scientist at the McDonnell Douglas Research Labs (1988-1992) and Edison Welding Institute (1992) before joining the faculty at The Ohio State University (1992-1999). Soboyejo spent a year (1997-1998) as a Visiting Martin Luther King Associate Professor at MIT before moving to Princeton University as a Professor (1999-2016).

He served as President and Provost of the African University of Science and Technology (AUST) between 2012 and 2014. Soboyejo moved to WPI in 2016 as the Bernard M. Gordon Dean of Engineering (2016-2018) and was later appointed as Senior Vice President and Provost (2018-2022). He is currently serving as Interim President of WPI. Soboyejo is the author of 4 text books and more than 400 peer-reviewed journal papers. He is also a member of the U.S. National Academy of Engineering, the World Academy of Science, the African Academy of Science, the Nigerian Academy of Science and the Nigerian Academy of Engineering.

11TH INTERNATIONAL CONFERENCE OF THE AFRICAN MATERIALS RESEARCH SOCIETY

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PLENARY SPEAKER



Prof. Malik Maaza

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Prof. M. Maaza is a native of North Africa, holds a PhD from the University of Paris-VI, is the current incumbent, in South Africa, of the UNESCO UNISA-ITLABS-NRF Africa Chair in Nanosciences. He is a joint staff of the University of South Africa and the National Research Foundation of South Africa.

He is a fellow of various Academies, including the African Academy of Science, the European Academy of Arts & Sciences as well as the National Academy of Science of India, the Islamic Academy of Sciences & the Royal Society of Chemistry-London. Prof. M. Maaza has been bestowed several awards & accolade among which; the African Union Nkwame Nkrumah award for Excellence in Science & Technology & the Galileo-Galilei award by the International Commission for Optics (ICO).

11TH INTERNATIONAL CONFERENCE OF THE AFRICAN MATERIALS RESEARCH SOCIETY

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PLENARY SPEAKER



Prof Maria Magdalena Titirici

Imperial College
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Magda Titirici is a Chair of Sustainable Energy Materials at Imperial College London and a Royal Academy of Engineering Chair in Emerging Technologies. Prior to Imperial Magda worked at the Max-Planck Institute of Colloids and Interfaces as a group leader and as a Reader/Professor at Queen Mary University of London.

Magda's research is in the area of sustainable materials for energy storage and conversion technologies, such as batteries beyond Li ion as well as fuel cells free of precious metals and H2 and sustainable chemicals from biomass/plastic waste electrolysis. Magda has published over 300 papers in this area and her research has been recognised by numerous awards such as the 2018 RSC Corday Morgan Prize and the 2020 Kavli Medal and Prize from the Royal Society.

11TH INTERNATIONAL CONFERENCE OF THE AFRICAN MATERIALS RESEARCH SOCIETY

Date: 12-15 December 2022
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PLENARY SPEAKER



Prof Malika Jeffries-EL

Boston University
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Malika Jeffries-EL is the Associate Dean of the Graduate School in Arts and Sciences and Associate Professor in the Department of Chemistry and Division of Materials Science at Boston University. She is also an Associate Editor for the Journal of Materials Chemistry C and the new RSC title Materials Advances. Dr. Jeffries-EL's research focuses on the development of organic semiconductors –materials that combine the processing properties of polymers with the electronic properties of semiconductors. She is a fellow of the American Chemical Society and the Royal Society of Chemistry and has won numerous awards including the Percy Julian Award from the National Organization of Black Chemist and Chemical Engineers (NOBCChE), the ACS-Women Chemist Committee Rising Star award, the Iota Sigma Pi Agnes Fay Morgan Award (2013). She has authored over 40 publications, received over 4000 citations, and given over 170 lectures domestically and abroad.

Professor Jeffries-EL, is also a staunch advocate for diversity and dedicated volunteer that has served in several activities within the American Chemical Society including the advisory board for the Women Chemist of Color Initiative and the Women Chemist Committee. She is a science communicator who seeks to encourage students from underrepresented groups to pursue STEM degrees an recently appeared on NOVA to talk about plastics. She also serves the community through her work with Alpha Kappa Alpha Sorority, Incorporated (AKA). Dr. Jeffries-EL is a native of Brooklyn, New York.

Website: https://africanmrs.net/senegal-2022/

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11TH INTERNATIONAL CONFERENCE OF THE AFRICAN MATERIALS RESEARCH SOCIETY

Date: 12-15 December 2022
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PLENARY SPEAKER



Prof Sossina M. Haile

Northwestern University
USA
Email: sossina.haile@northwestern.edu

Sossina M. Haile is the Walter P. Murphy Professor of Materials Science and Engineering at Northwestern University. She earned her Ph.D. in Materials Science and Engineering from the Massachusetts Institute of Technology in 1992. Haile's research broadly encompasses materials, especially oxides, for sustainable electrochemical energy technologies. She has published over 200 articles and holds 14 patents on these and other topics. Amongst her many awards, in 2008 Haile received an American Competitiveness and Innovation Fellowship from the U.S. National Science Foundation and in 2020 she was awarded the Turnbull Lectureship of the Materials Research Society. She is a fellow of the Materials Research Society, the American Ceramics Society, and the African Academy of Sciences, and a corresponding fellow of the Ethiopian Academy of Sciences.

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For inquiries
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Date: 12-15 December 2022
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PLENARY SPEAKER



Prof. Mamadou Diallo
National Science Foundation (NSF), Alexandria
USA
Email: mdiallo@nsf.gov

Prof. Mamadou Diallo was trained both as a chemical/environmental engineer and a physical chemist. He earned a Doctorate (PhD) in Environmental Engineering from the University of Michigan (U-M), a Master of Science (MSc) in Chemistry from U-M, an MSc in Chemical Engineering from Colorado School of Mines, and an Engineer Diploma (Ingénieur des Mines) from L 'Ecole Nationale Supérieure des Mines de Rabat (ENSMR). Prof. Diallo also completed post-doctoral training in Computational Chemistry at the California Institute of Technology (Caltech).

Since May 2020, Diallo has been serving as the Environmental Engineering Program Director in the Division of Chemical, Bioengineering, Environmental and Transport Systems (CBET) of the Directorate for Engineering at the National Science Foundation (NSF) in Alexandria (VA), USA. In addition to directing the NSF Environmental Engineering Program, Diallo is also serving as the Lead Program Director for the ELiS (Engineered Living Systems) Topic of the NSF FY22/F23 EFRI (Emerging Frontiers in Research and Innovation) Solicitation. At NSF, Diallo is also a member of the teams of program directors that are managing the PIPP (Predictive Intelligence for Pandemic Prevention) and the NNA (Navigating the New Artic) programs.

Prior to joining NSF, Prof. Diallo served as a Professorial Faculty in the Graduate School of EEWS (Energy, Environment, Water and Sustainability) at the Korea Advanced Institute of Science and Technology (KAIST) in Daejeon (South Korea) and a Research Faculty in the Caltech Divisions of EAS (Engineering and Applied Science) and CCE (Chemistry and Chemical Engineering). During the last 15 years, Diallo, his graduate students, and post-doctoral/faculty collaborators at KAIST and Caltech have been pioneering the development of a new family of mixed matrix membranes with in-situ synthesized polymer particles using dendrimers and hyperbranched polymers as building blocks. These membranes can be designed and tailored for a broad range of applications including 1) water purification, 2) metal extraction and recovery, 3) catalysis, and 4) downstream bioprocessing for the separation and purification of protein therapeutics. In 2015, Diallo's paper "Mining Critical Metals and Elements from Seawater: Opportunities and Challenges" was selected as the Best Feature article by the journal Environmental Science & Technology (ES&T) published by the American Chemical Society (ACS) [Available online at https://pubs.acs.org/doi/10.1021/acs.est.6b01454].

In addition to his NSF responsibilities and research activities, Diallo continues to serve as an Associate Editor of the Journal of Nanoparticle Research. More recently, Diallo served as a 1) a member of the Science Advisory Board (SAB) of the NSF ERC Nanotechnology-Enabled Water Treatment (NEWT) Engineering Research Center led by Rice University, 2) a member of the SAB of the Critical Materials Institute, a DOE Hub led by Ames National Laboratory, and 3) a consultant and advisor of the World Bank funded Africa Centers of Excellence Higher Education Project.



SYMPOSIUM-01
MATERIALS FOR CONSTRUCTION, MINING AND MANUFACTURING



KEYNOTE SPEAKERS



Prof. Lesley Cornish *is currently the Director: ARUA Centre of Excellence in Materials, Energy and Nanotechnology (CoE-MEN) as well as the Director of the DSI-NRF Centre of Excellence in Strong Materials, and Professor in the School of Chemical and Metallurgical Engineering, University of the Witwatersrand, Johannesburg, South Africa. She is is a Physical Metallurgist and her main research interests are phase equilibria and the development of alloys, especially platinum-based alloys for high temperature use in aggressive environments, and titanium-based alloys for potential dental applications. Her research also includes characterisation techniques, and well as mechanical properties and corrosion. She obtained her BSc (Metallurgy and Materials), MSc (Computer Science), PhD (Metallurgy and Materials) from the University of Birmingham, UK, and her Postgraduate Diploma in Education, cum laude from Wits. She has worked for the United Kingdom Atomic Energy Authority, University of the Witwatersrand and Mintek.*

Prof. Cornish is currently supervising or co-supervising 12 post graduate students, mainly at the University of the Witwatersrand, with 36 MSc and 29 PhD students already graduated. She has lectured to all undergraduate years in Metallurgical Engineering since 1990, postgraduate courses, and has given external courses on phase diagrams, heat treatment and lectures in the UK, USA, Zimbabwe, Botswana, Germany and Nigeria, as well as courses to De Beers, Mintek, and Necsa in South Africa.

She has won several awards at the Microscopy Society of Southern Africa (MSSA) Conference and won the (University of the Witwatersrand) Vice-Chancellor's Teaching Award in 1998, and Supervision Award: Faculty of Engineering and the Built Environment in 2015. She became a Fellow of the Royal Society of South Africa in 2010, and a Fellow of the South African Academy of Engineers (SAAE) in 2021. She was part of the team that was a R&D Magazine 2011, R&D 100 Winner, for Novel platinum/chromium alloy for the manufacture of improved coronary stents, for work done at Mintek; and won the National Science and Technology Forum "Eskom Research Capacity Award", 2013; as well as being in the team that won the "Communication and Outreach for Creating Awareness Award", with Profs. A. Quandt and D. Naidoo, and Ms C.K. Sparkes, in the National Science and Technology Forum-South32 Awards, 2016 – 2017. She was Second runner-up for Distinguished Women Researchers Natural (Physical and Life) and Engineering Science South African Women in Science in 2019.

Prof. Cornish has over 150 papers in refereed journals, as well as over 250 conference proceedings, 2 book chapters, and over 60 technical reports. She has been a member of the Materials Science International Team since 2000, and as well as the 34 phase diagram reviews published in books, she has also published about 30 system reports on the MSI website.

She regularly reviews papers for local and international journals and is a Member of the Editorial Board of Journal of Mining and Metallurgy B, and the International Journal of Refractory Metals and Hard Materials. She has been a Committee Member for both local and overseas conferences.

Titanium-Based Alloys with Copper Additions Targeted for Dental Applications

LESLEY A. CORNISH

School of Chemical and Metallurgical Engineering, University of the Witwatersrand,Johannesburg, South Africa, DST-NRF Centre of Excellence in Strong Materials, hosted by the University of the Witwatersrand, Johannesburg, South Africa, and African Research Universities Association (ARUA) Centre of Excellence in Materials, Energyand Nanotechnology (CoE-MEN)

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One of the most used alloys in dentistry is Ti-6Al-4V which comprises □□□ phases (hcp and bcc)and has very good properties. However, there have been concerns for the long-term use of this alloy because of reported toxicity the Al and V components, which may be detrimental. The Ti– 10.1Ta–1.7Nb–1.6Zr (wt%) alloy had already been developed by a collaborator and had demonstrated excellent osseointegration. A major problem in dental implants is peri-implantitus which is caused by the buildup of malignant bacteria that form a biofilm, leading to disease and loss of bone if not treated properly. One way to stop the biofilms is to add copper to the materialsused since copper has excellent antimicrobial properties. The research started by adding differentamounts of copper to Ti–10.1Ta–1.7Nb–1.6Zr (wt%) and the microstructures, hardnesses, and antimicrobial properties were derived. Similar work is underway on the Ti-10Ta-1.6Zr (wt%) alloy. Different composition binary titanium-copper alloys were also made and studied to attempt identification of the underlying effects for the antimicrobial properties, as well as tostudy the corrosion resistance, and to verify the Ti-Cu phase diagram on the Ti-rich side, for which there are many versions. Several different □□□ alloys with copper were also made after using Thermo-Calc to ascertain the two-phase structure, to find a less expensive alloy with good properties. The microstructures of these alloys were studied with SEM-EDX and XRD, and hardness and corrosion tests were done. Similar work is also being done on near-□ alloys with copper additions.

Keywords: Titanium, copper, dental application, phase diagram



Wolfram Schmidt *was born in Cologne, Germany. He received a diploma in structural engineering at the RWTH Aachen, Germany, and he holds a PhD in civil engineering from the Eindhoven University of Technology, Netherlands. Wolfram Schmidt works at in the department "Safety of Structures" at BAM, responsible for the research group that works in the rheology and admixture laboratory with a research focus on particle-polymer-fluid interactions and innovative organic and mineral cement and concrete constituents. Furthermore, he is Secretary of the German Rheological Society (DRG), and member of the International Federation for Structural Concrete (fib). In the International Union of Laboratories and Experts in Construction Materials, Systems and Structures (RILEM), he is Officer in the Development Advisory Committee and Bureau. In RILEM he has also been member of different Technical Committees on rheology and sustainable cement-based solutions and the Educational Activities Committee, and he is also the Convenor for the sub-Saharan African region. Within the framework of fib and RILEM activities, he has been among the drivers to implement the GLOBE Global Consensus on Sustainability in the Built Environment, but he is also involved in a variety of other international initiatives related to sustainable construction, including policy advice and standardization activities.*

He is founder of the Pan-African cement round robin (PACE-PTS) and initiator of the conference series "Advances in Cement and Concrete Technology in Africa" (ACCTA) and ISEE-Africa (Innovation, Science, Engineering, Education). With his colleague Kolawole Olonade (UNILAG) he received the German-African Innovation Incentive Award GAIIA of the German Federal Ministry of Education and Research for developing cementitious binders and chemical admixtures from wastes of cassava production. In this context, it was possible to build the first real-size structure where large part of the Portland cement in concrete were replaced by sustainable cassava peel ash.

Many of his research and educational projects such as KEYS, INFRACOST, and Local-Care are focused on the potentials for more sustainable, circular urban construction technologies using local, environmentally friendly resources in Africa. In this context, he has recently initiated the Female Academic Leadership Network for Conscious Engineering and Science towards Sustainable Urbanisation (FALCONESS).

Future-Oriented Standards for Cement, Admixtures, and Concrete – How Africa Can Spearhead the Implementation of Green Urban Construction Materials

WOLFRAM SCHMIDT

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There is no alternative to concrete when it comes to infrastructure and urban construction materials. In comparison, to other structural mass materials, it has a low carbon footprint and it is the only material that can meet the global demand. However, since it is the most widely used commodity in the world after water, its production is responsible for 10-15% of the global carbon emissions. The major contributor to the carbon footprint of concrete is its binder, Portland cement, which alone is responsible for about 8% of the total anthropogenic carbon emissions. Therefore, future materials developments have to focus on using concrete with less Portland cement and using the binder in concrete more efficiently. Novel binder concepts, for example based on calcined clay, agricultural waste ashes or natural resources do exist, and a variety of construction chemicals can support their implementation and optimum usage. However, the existing standards frameworks all over the world are not ready for the effective implementation, since cement and concrete standards are based on very traditional concrete mixture compositions, and raw materials sources that are running out today. In addition, even though the chemical agents of chemical concrete admixtures are following standards, their very elementary interaction with the early cement hydration is not covered in any standard all over the world. The paper highlights the shortcomings of existing cement, concrete and admixture standards and provides performance and reaction-based solutions how to make the standards framework capable of dealing with today's construction challenges and the yet unknown challenges of the future. Particularly in Africa, where urbanization takes place at rapid pace, a disruptive change of the standardization framework can support the continents potential to become green construction pioneer.



Karen Scrivener *has been Professor and Director of the Laboratory of Construction Materials in the Department of Materials of EPFL (Ecole Polytechnique Federale de Lausanne for the last 20 years. She is a Fellow of the UK Royal Academy of Engineering and author of over 200 journal papers.*

Her research focusses on the understanding the chemistry and microstructure of cement-based materials and improving their sustainability. In 2008, she came up with the idea for LC3 cement, this material has the potential to cut CO2 emissions related to cement by more than 400 million tonnes a year.
She received her bachelor's degree in Materials Science from the University of Cambridge in 1979 and her PhD from Imperial College London in 1984.

Practical Solutions to Reduce Embodied CO2 in Construction

KAREN SCRIVENER

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Increasing attention is focussing on the CO2 associated with construction. Worldwide around 20% - 25% of emissions can be linked to construction and about one third of these come from cement. However, cement as used in concrete has lower emissions than almost any other building material – the high impact comes only from the enormous amounts used. I will talk about practical possibilities to reduce these emissions, which can be implemented worldwide and at large scale. One of the two most important possibilities are the potential to replace a large part of clinker with a combination of calcined clay and limestone in LC3 technology. The other is to move towards more industrial ways of producing concrete in ready mix plants, rather than on-site mixing from cement in bags.



EARLY CAREERS - SPEAKERS



Dr. Khadim NDIAYE *is an Associate Professor at the Laboratory of Mechanics and Materials of Civil Engineering (L2MGC), Department of Civil Engineering, CY Cergy Paris University, France. He holds a Master's degree in Civil Engineering and obtained a PhD at the Toulouse University (LMDC INSA Toulouse – UPS). The L2MGC is structured into four thematic research centers focusing on Rheology, Mechanics of Materials and Structures, Durability and Auscultation, and Thermo-Hydro-Chemo-Mechanical behavior (THCM).*

His research interest focuses on the development of innovative and low-impact cementitious materials, physicochemical characterization, thermodynamic modelling of hydration, durability of cements-based materials and heat storage concretes. He is one of France's pioneers in the field of heat storage by cementitious materials with a patent application. Since joining the L2MGC in 2018, he has been developing the line of research on the elaboration and durability of alkaline activated industrial by-products (slag, flay ash, metakaolin, sediments) and compressed earth blocks.
Currently, Dr. Khadim NDIAYE is supervising 4 thesis:

- *Valorization of dredged sediments in manufacturing compressed earth blocks stabilized by alkali-activated fly ash binder.*
- *Elaboration of an eco-binder/geopolymer based on industrial by-products – application for the formulation of reinforced concrete and road materials.*
- *Development of materials based on raw earth intended for the public works.*
- *Study of a binder based on alkaline activated limestone.*

Experimental Study on Effects of Concrete Hydric State on Its Carbonation Depth

KHADIM NDIAYE[1], YANNICK FEUTSEU[1], MENGYA LI[1], BRUNO FIORO[1], JEAN-LOUIS GALLIAS[1]

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The construction sector has huge environmental and socioeconomic impacts. It is one of the largest exploiters of resources, with half of them being non-renewable. According to the World Watch Institute, the industry consumes 40% of the world's usage in raw stones, gravel and sand. The improvement of concrete durability allows to increase the lifetime of concrete structures, and thus to reduce their carbon footprint. Carbonation of concrete is the major time-limiting factor for the durability of reinforced concrete structures. The CO_2 from the air penetrates into concrete through pores and reacts with calcium hydroxide to form calcium carbonates destroying the high pH environment of surrounding concrete which protects the steel bars of reinforced concrete from corrosion. Many parameters influencing carbonation depth have been widely studied: temperature, CO_2 concentration, cement type, permeability, cure condition and environmental relative humidity. The latter has a significant influence on the carbonation depth. It is well known that the carbonation kinetics is heavily dependent on environmental conditions of the concrete. However, there is a real lack of scientific literature about the local hydric state effect on carbonation depth. The objective of this study is to investigate the relation between carbonation depth and local hydric state of the concrete in order to better control the lifetime of concrete structures. The results of accelerated carbonation tests confirm that the carbonation front moves towards drying front over time.

Keywords: Concrete, Durability, Carbonation depth, Drying depth



Dr Walid Yahiaoui *got his engineering degree at the civil engineering department, University Saâd Dahleb-Blida 1 in Algeria in 2010. He pursued his MPhil degree in 2013 at the same university working on the effect of local aggressive environments on the performance of ordinary concrete. He obtained his doctorate in 2018 at the same university on the effect of hot climate on self-compacting concrete with blast furnace slag as cement replacement.*

He is currently a lecturer at the university of Blida1 giving courses on novel and eco-friendly materials as well as on reinforced concrete. His main interests include recycling, cement replacement materials and natural fibers in cementitious materials. He has published about ten publications in international journals and international conferences.

Performance of Eco-Repair Mortar Based on Waste Brick Fines

YAHIAOUI WALID [1*], MENADI BELKACEM [1], KENAI SAID [1], BENSACI HAMZA[1]

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After several years of use of structures, many concrete structures are damaged by mechanical, chemical and physical attacks or by the corrosion of the reinforcements. This requires repairs to increase structures life. On the other hand, the reduction of global warming is actually one of the priorities that promotes the production of low-carbon concrete with low environmental impact. This study aims to develop an environment friendly repair mortar based on brick waste fines and natural fibers. For this purpose, the effect of partial substitution of cement with brick waste fines (BWF) at a content of 5%, 10% and 15% and the addition of 1% of alfa fibers of the total volume with 10 mm length on the performance of a repair mortar were investigated. The vegetable fibers (Alfa) were treated by 6% of NaOH and boiling water. The properties studied include, compressive strength, flexural strength, the pull-off, slant shear and thermal conductivity. The results obtained showed that the repair mortar samples containing treated alfa fibers by boiling water or alkaline treatment, enhances the properties of the flexural strength, pull-off adhesion, slant shear stress and thermal conductivity at the age of 90 days.

Keywords: Repair mortar, brick waste fines, alfa fiber, strength, slant shear, pull-off adhesion, thermal conductivity.



Philbert NSHIMIYIMANA *is lecturer-researcher in civil engineering at Institute 2iE [International institute for water and environmental engineering] in Burkina Faso.*
He earnt his engineering degree in Materials Science and Engineering in 2016 at AUST [African University of Science and Technology] in Nigeria and a sandwich PhD degree in building Materials in 2020 at both Institute 2iE and University of Liege, Belgium.
After completing his PhD, he has been teaching materials-oriented classes such as chemistry of solid, hydraulic binders and Eco-Materials, and concrete technology and reinforced concrete at Institute 2iE.
His primary research interests evolved around clean building materials and sustainable constructions: from raw earth-based materials to the improvement of their thermal-energy and durability performances for building constructions; from the value addition of by-products to the elaboration of low carbon cementitious materials and concrete.
Philbert NSHIMIYIMANA is currently a member of RILEM [International Union of Laboratories and Experts in Construction Materials, Systems and Structures]'s technical committee MAE: [Mechanical performance and durability assessment of earthen elements and structures] which aims to define dedicated testing procedures for stabilized and unstabilized earth as a building construction material.
His research publication at https://www.researchgate.net/profile/Philbert-Nshimiyimana
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[Laboratoire Eco-Matériaux et Habitats Durables- Institut International de l'Ingénierie de l'Eau et de l'Environnement]

Improving the Performances of Compressed Earth Blocks by Stabilization Using Alternative Binders

PHILBERT NSHIMIYIMANA [a, *], ADAMAH MESSAN [a], LUC COURARD [b]

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The alternative construction materials are promising for the applications in the modern constructions for abiding by environmental sustainability and circular economy. Clay earthen materials are the most common building materials used all over the world. The suitability of these materials is characterized for the production of stabilized compressed earth blocks (CEBs) for applications in building construction, specifically in the Sahelian climatic context. Industrial by-products: lime-rich residue (lime) and agricultural by-products: amorphous silica–rich rice husk ash (ash) are also characterized for the stabilization of CEBs. Mixtures were produced by addition of 0-25 wt% lime, 10-25 wt% lime:ash (various ratios) to the earthen materials. The mixtures were used to produce the mix solutions, for monitoring the reactivity of materials, and mold stabilized CEBs (295x140x95 mm^3) for testing the physico-mechanical, thermal and durability performances of CEBs. The results show that the earthen material which contains a relatively high fraction of poorly ordered kaolinite clay mineral records the highest pozzolanic reactivity with lime than material that contains high fraction of quartz mineral. The compressive strength of CEBs stabilized with 20% lime improved tenfold (from 0.8 to 8.3 MPa) with the most reactive material; compared to the improvement of only two-fold (from 2 to 7.1 MPa) with the least reactive material. These materials are suitable for the production of stabilized CEBs with the compressive strength greater than 4 MPa. Moreover, the stabilization of the earthen material improved the structural efficiency of CEBs: increase of compressive strength and decrease of bulk density, as well as the thermal efficiency: decrease of thermal effusivity, conductivity and diffusivity and increase of thermal specific capacity. It also improved the indicators of durability in time of CEBs: increase of the stability in liquid water, resistance to abrasion and resistance to erosion. Therefore, the CEBs stabilized with by-product alternative binders satisfy engineering requirements and durability performances for the construction of load-bearing and facing masonry.

Keywords: lime residue; compressed earth block; durability; kaolinite clay; pozzolanic reactivity; physico-mechanical property, rice husk ash.



INVITED SPEAKERS

Agrowaste in Cementitious Materials for an Environment Friendly Concrete

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Concrete is the most widely used material in the world after water. However, concrete contribute to about 10% of global carbon emissions. One of the solutions to reduce its carbon footprint, is to use waste materials either as a substitution to aggregates or to cement. Agro-waste materials in the form of powders or fibers are renewable and are widely available and could be used in cement mortar in various applications in the construction sector.
In this paper, the use of different agro-waste materials in cement mortar is reviewed. Some experimental data on the mechanical and durability performance of mortars based on date palm fibers, alpha fibers and cork in combination with local mineral additions (slag and natural pozzolan) is also presented.
The experimental results showed that the mechanical and durability performances of mortars with agro-waste fibers were comparable to those of imported readymade mortars and could be used successfully as repair mortar. The use of cork as aggregates produced a lightweight mortar with good insulation properties.

Keywords: agrowaste, carbon emission, fibers, mortar, concrete.

An Overview of Bio-Waste Materials as Precursors for Alkali Activated Cement

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Indisputably, climate change remains the major challenge in the 21st Century. This is due to unprecedented emission of greenhouse gases (GHG) to the atmosphere as a result of human activities, causing depletion of ozone layer; hence global warming. Cement production is implicated as a major emitter of carbon dioxide. In order to achieve zero emission in the year 2050 as targeted, there is urgent need to find alternative to Portland cement. One of such alternatives is alkali activated cement. Different industrial wastes have been found to be suitableprecursors for alkali activation. Nevertheless, there is dearth of information on the use of bio- wastes. In this paper, common bio-based materials are exam&ined for possible use as precursor. Properties of each of the selected bio-wastes are x-rayed with a view to understanding their performance. Processing techniques adopted for activation as well as the mechanism of alkali activation is presented. The challenges for use of these materials are equally assessed, while suggestions on how to fully utilized the materials are underscored, especially in Africa where these materials are abundantly available.

CARBON NANOTUBES DISPERSION STRENGTHENING OF NICKEL ALUMINIDE

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As the competitive global technological development is increasingly advancing, materials engineers are constantly confronted with the challenge to develop innovative materials with improved properties for the rapidly evolving and wide range of technological applications. The lightweight and unique properties of nickel aluminides (NiAl) such as, high oxidation resistance, high strength and wear resistance at elevated temperatures have attracted different players in the materials engineering research endeavours to exploring these materials in competitive cutting-edge applications over existing nickel-based superalloys. Nevertheless, the commercialization of NiAl has been limited owing to their low plasticity, lack of ambient temperature toughness and poor fracture toughness. To improve the ambient temperature low ductility and fracture toughness that limits the wider applications of these alloys, we focused our attention in this project on investigating unique technique for uniform dispersion of carbon nanotubes within the matrices of these alloys and understanding their structural and phase transformations during spark plasma sintering.

The Production and Application of Ferrous Metal Matrix Composites for Mining Components

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Wear-resistant materials are used in a number of industrial processes to prevent or reduce wear loss and reduce downtime of equipment operating in abrasive environments, and to enhance performance and quality. When hard metals and steels are used, especially at high velocities and pressures, or when the working parts are subjected to high temperatures and thermal shocks, they can be quickly destroyed, especially when transported in liquid corrosive environments.
The purpose of this study was to investigate the use of a ceramic metal matrix to improve wear resistance. Mineral and mining industries have a growing application potential for engineering ceramics for wear and corrosion protection of extraction, processing, conveying, dust collection, and piping systems. The use of innovative metal-matrix composites made from non-ferrous metals has been widely researched and developed. Creating composites using ferrous alloys presents monumental challenges for casting. It is first necessary to realize that the density differential produces large buoyant forces on the ceramic, resulting in the ceramic float on the metal stream unless a rigid structure is incorporated. Secondly, the poor wetting properties of the metal and ceramic will lead to inferior bonding of the matrix, resulting in solid separation in service. In the current study, ceramic-based compositions were infiltrated into a ferrous matrix. Filters and rods made of Alumina (Al_2O_3) were used. When the hot metal was in contact with the cold alumina rods in the mold, the rods cracked. Alumina floats under Ferro static pressure because of the density difference between ceramics and liquid metals. The amount of liquid metal infiltrating ceramic filters increased with the amount of pores per linear inch (ppi), which is measured as pore volume fraction. As a result, casting with 10ppi was found to have a high infiltration rate, followed by 30ppi, and ceramics with 50ppi had a poor infiltration rate. The infiltration rate of ceramics increased with increasing temperature.

Keywords: Metal Matrix Composite, Wear Resistance, Ferrous Matrix

Characterization and Performance of Refunctionalized $LiFePO_4$ Cathodes Harvested from a Hybrid-Electric Bus Battery

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Lithium-ion batteries (LIBs) in Sub-Saharan Africa is projected to grow over 750% between 2020 and 2030.[1] A circular economy for LIBs in the region would have two key benefits: (1) supporting the sustainable supply of battery materials by complementing and reducing the societal pressures of mining industries, and (2) managing significant safety hazards of LIB waste (e.g., fires and environmental contamination). Recycling facilities are a crucial component of circular economies and require the development of technologies, infrastructure, and regulations to fill the gap between recycling needs and capacity.

Is there a need for a better understanding of the factors that influence the performance of active battery materials after direct recycling processes, in which the crystal structure is preserved and functionally restored. Furthermore, the scalability of such methods must be further developed to take advantage of the potential environmental benefits of direct recycling as a battery waste management practice.

The primary aim in this work is to develop and evaluate direct-recycling methods for $LiFePO_4$ (LFP). LFP is projected to play an important role in future LIB markets due to low cost and high safety. Furthermore, it lacks valuable materials like cobalt and nickel, making traditional recycling methods like hydro- and pyrometallurgical extraction economically infeasible.

The existing literature on direct-recycling LFP focuses on lab-aged cells with consistent states-of-health. In this work, we implemented relithiation experiments on six cylindrical 26650 cells harvested from a retired hybrid-electric city bus. The cells were originally manufactured between 2009 and 2017 by A123. The percent of the initial capacity of the recycled cells ranged from 10% to 90%. Cathode materials were characterized before and after relithiation using constant-current cycling, XRD, and SEM. In this talk, we will summarize the dependency between the pre-recycling state-of-health and the electrochemical performance and properties of the recycled cathode material.

Keywords: lithium-ion batteries, direct-recycling, refunctionalization, relithiation

The Potential Use of Waste Materials as Admixtures in Concrete Technologies

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Admixtures have highly contributed to the development of concrete performance over the latest decades. This can explain why admixture market is a constant increase in Africa and in developing regions. Moreover, the highest costs of concrete are found in Africa mainly because admixtures are often not produced on the continent. Besides, African economy remains based on the agriculture and agriculture produces an important amount of unused waste. The article deals with the potential use of some of these agro-waste materials in concrete technology. Three of them were presented, Acacia gum, nkui sap and knikeliba sap. Preliminary results show that the gum acts like a superplasticiser, while the sap gives a thixotropic behaviour to fresh cement. Though the outcomes on the kinkeliba are not clear, this sap tend to develop glue properties when it is exposed to the air.

Comparative analysis of Bentonites from African and Asian Sources for the Manufacture of Castings

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Abstract Text: Bentonite Bentonite is an essential commodity in the foundry industry. Bentonite is a clay mineral with high montmorillonite content used as a bonding agent in greensand moulding process. Castings such as steering knuckles, brake drums, hubs and ventilated disc are typical examples of goods manufactured from the greensand process. The main mineral in bentonite is montmorillonite which is generally classified as sodium Na. or calcium Ca. types, depending on which exchangeable ion is dominant. Five bentonite samples from different African and Asian sources were evaluated by various techniques to determine their physical and chemical properties and to compare their strength mechanisms. Testing included measurement of cation capacity exchange (CEC), pH, swelling index, viscosity, chemical composition, mineralogy, green compression strength, shear strength, wet tensile. Thermal stability tests, were also taken for each bentonite from different sources at two different temperatures, firstly at 500ºC and at 600ºC. According to the results, the properties of the five bentonites tested fall within the specification of the foundry industry. According to thermal stability results, the five bentonites increase their green strength when heated at 500ºC. However, it was found that at the temperature of 600ºC bentonite from supplier A in Africa did not have a huge reduction in strength as compared to other bentonites. The results in this research show how the mulling time has an influence on the strength of each bentonite.



ORAL PRESENTATERS

Application of Composites Modified CNTS Nanotubes for Concrete Bridge Reinforcement- Numerical Analysis

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Composite materials have been used for more than thirty years as a repair and/or reinforcement technique for concrete structures, particularly bridges and elevated structures. Despite their effectiveness and ease of implementation and other advantages, the problem of disbonding of composite plates/fibers from the surface of the concrete support sometimes arises, especially in high temperature climates. In this paper we propose, a numerical analysis based on the finite element method, of an old reinforced concrete bridge, located at 65km from the capital Algiers, reinforced by application of carbon fiber based bonded composites (CFRP), with the insertion of carbon nanotube powders (CNTs) in the resin used, with percentages of 0%, 0.5%, 1% and 2%. The results of a modal analysis (before and after reinforcement), showed that these nano-composites (CNTs) improve the mechanical performances of the epoxy resin and consequently those of the composite material (CFRP) applied and give appreciable gains at the vibration frequencies, of the order of 25 to 65%, of the various modes of the tested bridge.

Keywords: concrete Bridge, composites, CNTs, reinforcement, numerical analysis.

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Investigation of Network Microstructure of Tib/Ti6Al4V Composite Manufactured with Laser Metal Deposition

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This work present microstructural investigation of in-situ synthesized TiB/Ti6Al4V composite that was manufactured with laser metal deposition (LMD) technique. Single track samples were manufactured at volumes of 0.1 rpm and 5.0 rpm for TiB_2 and Ti6Al4V, respectively, and were characterized for microstructure and hardness. It was found that the network microstructure and forms two different morphologies on the samples, with equiaxed and columnar grains preferably forming on the top and bottom regions, respectively, due heat travelling direction during the LMD process. In addition, the hardness increased from 368 ± 7HV to 505 ± 16HV with addition of TiB_2.

Keywords: Titanium matrix composites, Laser metal deposition, Microstructure.

Pitting Corrosion Susceptibility of Nickel-Silica Ni-SiO_2 Electrodeposited Composite Coatings on Carbon Steel Assessed Through Syringe Cell Technic in 0.6 M NaCl

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Corrosion prevention remains a challenge for governments so that billions are spent as well as to support research and to maintain equipment in good state. In chloride salt environments, steel many and other metal compositions may undergo pitting corrosion [1]. This research deals with the assessment of pitting corrosion of nickel silica composites electrodeposited coating [2]by the mean of the syringe cell [3]. The interpretations of potentiodynamic curves in Tafel plot indicate that corrosion potential increases from -456 mV of carbon steel to values up to -205 mV for steel reinforced nickel-silica coatings. The pitting potential also increases in the same order to +187 mV for composite coatings contrary to that of carbon steel which is -201 mV.
Results show that pitting corrosion susceptibility is a function of heterogeneity induced in the composite material due to the presence of silica particles leading to pits depths of about 70 microns determined by the mean of optical profilometry.

Keywords: Pitting corrosion; composite coating; Silica

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Effect of Preheat on Mechanical Properties of Nitinol (NiTiNb) Manufacture Using Laser Cladding Process

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Laser direct metal deposition technique (LDMD) was used to produce Nitinol (NiTi) alloy that contained trace of Niobium (Nb). While NiTi is known of its good superelasticity, shape memory effect, low stiffness, and good corrosion resistance, the addition of Nb in small amount(s) into a NiTi matrix with 50 at. % of both titanium (Ti) and nickel (Ni) lead to an improvement in the mechanical properties of Nitinol. In this study, LDMD was used to 3D print cubes of about 20*20*20 mm^3 from a mechanically pre-alloyed powder consisting of $Ti_{52.5}Ni_{42.5}Nb_{7.5}$ on a preheated Ti6Al4V base plate. Preheat temperatures were varied from 300°C, 500°C and 700°C. The fabricated cubes were characterized using appearance using optical microscope (OM), and for composition and high-resolution imaging using scanning electron microscope equipped with energy dispersive X-ray spectroscope (SEM-EDS). The mechanical performance test were conducted using Vickers' micro-hardness machine, nano-indentation hardness machine, compression tester and wear tester. Results concluded a decrease in hardness and compressive strength with an increase Temperature.

Novel 3d-Printable Carbonated Polymer (Carbopolys) Composite

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Carbonated polymer composites (CarboPolys), first synthesized by our research team using forced carbonation, have the potential to be utilized as carbon dioxide (CO_2) storage and phase transformation mediums. However, to be successfully applicable, control and optimization in the synthesis of these composite materials are required. In this study, we utilize an automated mechanism to synthesize CarboPolys via microbubble generation and diffusion. The properties of this material and subsequent manufactured parts are dependent on microbubble average size range, volume fraction, and distribution within the polymer matrix. Viscosity measurements revealed that for the neat resin, at low temperatures, the dynamic viscosity is initially at a high value of 7mm^2/s. However, with increasing temperature up to 100ºC it shows a steady decrease in the viscosity with no signs of polymerization. The CarboPoly exhibited a similar trend with the exception that at a moderate volume fraction carbonation loading, its initial viscosity was lower. It was also found that the size of the microbubbles was affected by temperature, with higher temperatures resulting in smaller bubbles on average. Lower resin viscosity facilitated the migration of the microbubbles throughout the resin resulting in an increase in bubble-in-matrix dispersion. We further set out to 3D print the CarboPolys to realize part resolution and structural complexity using digital light projection (DLP). Printing resolution tests were performed using structural and dimensional variation parameters. Thermo-mechanical characterization of the 3D-printed CarboPoly parts were carried out. An initial increase in polymer carbonation duration showed a 16% increase in porosity, more stable thermal profiles, and a 40% decrease in specific heat capacity. Thermo-mechanical compressive tests on an optimum carbonated sample revealed a 70% increase in compressive strength over its neat counterpart and a peak modulus at 50 °C of 60 MPa.

Keywords: Carbonated Composites, Additive Manufacturing, 3D-Printing, Thermo-Mechanical Characterization

Peformance of Alkali-Activated Rice Husk Ash Concretes in Aggressive Chloride Environment

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The study investigated the effect of alkali activated rice husk ash in chloride environment. Sodium hydroxide (NaOH) and sodium metasilicate (Na_2SiO_3) were used to prepare the alkali activated binder, at a ratio of 1:2 and rice husk ash was added at 5%, intervals. Concrete mix of 1:1.6:2.6 and size 100 mm x 100 mm x 100mm made with different percentages of RHA (0%, 5%, 10% and 15 % by weight of cement) were cast with water-cement ratio of 0.5. A total of 96 cubes were cast cured for compressive strength tests at 7, 28, 56 and 90 days respectively. Two chloride environments to mimic Ocean and Lagoon (18618.05mg/L and 24878.80mg/L) environments respectively used for chloride penetration test. 16 cubes were cast for chloride penetration test for each environment at 0%, 5%, 10% and 15% at 56 and 90 days. The test was carried out by slicing the concretes at 12.5, 20, 27.5, 35, 42.5 and 50 mm depths. The sliced samples were pounded and mixed with distilled water and titrated in the laboratory to measure the chloride concentration at each depth. The compressive strength results in 18618.05mg/L and 24878.80mg/L media for control at 56 and 90 days are (32.05N/mm^2 and 30.60N/mm^2) and (31.04N/mm^2 and 29.09N/mm^2) respectively. The compressive strength results in 18618.05mg/L medium for 5%, 10%, 15% RHA at 56 and 90 days are (22.53N/mm^2, 27.04N/mm^2 and 31.14N/mm^2) and (24.58N/mm^2, 29.60N/mm^2 and 34.19N/mm^2) respectively. For 24878.80mg/L medium at 56 and 90 days (21.68N/mm^2, 26.14N/mm^2 and 30.15N/mm^2) and (23.23N/mm^2, 28.19 N/mm^2 and 32.70 N/mm^2) respectively. The chloride penetration test at 90 days for control, 5%, 10% and 15% RHA in 18618.05mg/L medium are (1040.37 mg/L, 908.32 mg/L, 277.27 mg/L and 218.42 mg/L) respectively and for (24878.80mg/L medium the results are (1190.31 mg/L, 1003.97 mg/L, 449.68 mg/L and 286.24 mg/L) respectively. It can be concluded that 15% RHA replacement compares well with control for both compressive strength and chloride penetration at 90 days.

Keywords: Alkali-activated material, rice husk ash (RHA), Chloride environments, Compressive strength, Chloride penetration

Influence of Shea Butter Residues on the Physical and Mechanical Properties of Earth Renders

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This paper studies the influence of shea butter residues on the microstructural physical and mechanical properties of earth renders. For this, a moderately plastic clay soil from Kôdéni (Burkina Faso) consisting of kaolinite (62 wt.%), quartz (31 wt.%) and goethite (2 wt.%) was used in manufacturing earth renders. The earth renders were reinforced with shea butter residues up to 6 wt.%. The mineralogical and microstructural characteristics of shea butter residues as well as the physical and mechanical properties of earth renders were evaluated. It emerges from this study that earth renders reinforced with shea butter residues offer better water resistance and good erosion resistance due to the presence of fatty substances (oils) in the shea butter residues which have hydrophobic properties as well as low thermal conductivity. The incorporation of shea butter residues into the clayey matrix increases abrasion resistance while flexural and compressive strengths decrease. This is due to accumulation of these shea butter residues in clayey matrix which creates internal pores in adobes. The manufactured earth renders considering to their good water resistance and low thermal conductivity are suitable for habitats in hot climate.

Keywords: Earth renders; Shea butter residues; Microstructural; Physical and mechanical properties; thermal comfort; water resistance.

Characterization of Heater-Cooler Blocks Fabricated from Aluminium Wastes for Steady-State Thermal Application

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Recycling aluminium (Al) from waste aluminium scraps for fabricating aluminium casts is a waste management technique suitable for reducing environmental pollution. The aluminium casts can be further processed into different materials of engineering interests, such as heater-cooler (thermal) blocks. In this study, the microstructural characterisation of aluminium cast fabricated from recycled aluminium waste and adapted for use via the (steady-state technique) as heater-cooler blocks required in the determination of the thermal conductivity of conducting solid composites was investigated. The characterization was investigated using Scanning Electron Microscopy (SEM), Energy Displacer Spectroscopy (EDS), X-ray Diffractometer (XRD), and X-ray Fluorescence (XRF). The XRD result confirms the crystalline structure of aluminium on the fabricated aluminium cast. The elemental composition results demonstrated that the fabricated cast contains 90% Al, with Silicon (Si) accounting for about 8% of the chemical composition. In comparison, the remaining 2% was contributed by C, O, Fe, Zn, and Cu. The compositional change observed during characterization was attributed to the recycling process used in fabricating the aluminium cast.

Keywords: Aluminium cast, aluminium scraps, heater-cooler blocks, thermal conductivity, steady state, recycling

Physical Analyzes Applied to Lateritic Soils of Western Senegal for their Geochemical, Mineralogical and Microstructural Identification

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Lateritic gravels are generally used materials in Building and Public Works without prior knowledge of their mineralogical and chemical composition that can significantly impact their geotechnical behavior. For mineralogical identification, X-ray diffraction which highlight mineral phases, Raman and infrared molecular spectroscopies, that make it possible to invalidate parasitic mineral phases are applied. Scanning electron microscopy (SEM) provides information on the microstructure of materials as well as their elemental chemical composition using the SEM with Energy Dispersive Spectroscopy technique.

Five borrow pits of lateritic gravels located in Thies and dynamically operated for the supply of road and highway construction sites in the Thies and Dakar regions in Senegal are studied. These are those of Lam-Lam, Mont-Rolland, Pout, Ngoundiane and Sindia. The Mineralogy results are common to all the borrow materials and specific to laterites. Materials are made up of quartz represented by sand, kaolinite by clay, goethite and hematite are the ferric oxides of particle bonds which allow the formation of aggregates of pisolitic nodules. Lateritic gravels are formed by this process in tropical areas subjected to leaching and precipitation of elements according to their ionic potential. The microstructure of these materials is marked by the presence of laminated clay and granular particles, frequently aggregated by the ferric minerals and thus leaving pores between them.

Stable minerals form these materials, poor in alkaline and alkaline-earth elements but rich in iron, aluminum and silica and of course in oxygen which guaranteeing the bonding of cations of coordination polyhedra that forming mineral phases. The microstructural examination allows to recognize the laminated structure of the kaolinitic clay, which is neither swelling and nor very sensitive to water, and pores which can be significantly reduced by mandatory compaction before the use of these materials in road construction.

Keywords: Thies, lateritic soils, mineralogy, spectroscopy, microstructure

Effect of Curing Conditions on the Physico-Mechanical Properties of a Metakaolin-Based Geopolymer Concrete Containing Calcium Carbide Residue

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Today, hydraulic concrete remains the most used construction material in spite of the very polluting character of its main binder, namely Portland cement. However, alternatives exist, such as geopolymer concretes. Current studies reported that the physical, mechanical and durability performances of these concretes can significantly be affected by the curing conditions, among other parameters. Previous studies have demonstrated that geopolymers reach better performances when they are cured at temperature approaching 60 °C. This can be a limit for in-situ application of such concrete. The present study aims to produce a geopolymer concrete under ambient conditions, i.e. cured at controlled temperature of 20±2 °C and uncontrolled ambient temperatures of 30-35°C. It specifically assesses the effect of curing temperature on the physico-mechanical properties of a geopolymer concrete. The metakaolin-based geopolymer concrete was designed by partial combination with an industrial by-product, namely calcium carbide residue (CCR), in the ratios of 5 to 25 wt% of metakaolin powder. The concrete was cured at two different temperatures (20 °C and 30 °C), which represent respectively the minimum and the average ambient temperature in the study region (Ouagadougou). The concrete was characterized in fresh state (workability, setting time, density) and hardened state (compressive strength, density) at 7, 14, 28 and 90 days. The results indicate that the curing temperature has a significant effect on the physico-mechanical properties of geopolymer concretes. Setting times are longer at 20°C (more than 2970 minutes) than at 30°C (less than 2500 minutes) for all designs. At 7 days, the compressive strength increased by 70% (3.1 MPa to 5.3 MPa) when cured from 20°C to 30°C for the concrete containing 10% CCR. At 28 days, the compressive strength increased by 29% (14.4 MPa to 18.6 MPa) when cured from 20°C to 30°C for the concrete containing 10% CCR. The values of the strength obtained at 30°C are relatively higher than those obtained at 20°C for all the curing age, respectively reaching the maximum values of 31 MPa and 14 MPa for concrete containing 15% CCR at 90 days.

Keywords: Ambient curing, Calcium carbide residue, Geopolymer concrete, Metakaolin, Physical and mechanical properties

Road Use of Diamniadio Swelling Soils

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A crossroads city located 30 km from Dakar in Rufisque department, DIAMNIADIO was chosen by the Senegalese authorities in 2012 to decongest Senegalese capital from economic activities and administrative services and respond to demographic and urbanization dynamics. The new town of Diam niadio covers 1,644 ha and should accommodate 350,000 inhabitants. Diamniadio aims to meet the requirements of a modern city comprising administrative districts, residential areas, industrial parks, universities, research centers and sports infrastructure.
The construction on site is a constraint by the nature of the soil. The Diamniadio basement is known for its retraction-swelling nature. It is a marly soil containing swelling clays which give it this character.
The main methods of foundation construction on swelling soil are deep foundations or the substitution of soil by compacted laterite or improved cement sand.
The excavated soil is stored and becomes construction waste for which no solution is applied.
The study relates to the use of the Diamniadio swelling marl in the construction of road infrastructures in road fill and subgrade.
The Sandly marl reconstituted in the laboratory is composed of 75% marl and 25% Sand 0/1
Sandly marl treated with 3% and 5% lime respectively meet the criteria for use in road fill and subgrade
The formulation study revealed a processability with swelling values of less than 5%, bearing values greater than 32 and a CBR/IPI Ratio greater than 1

Keywords: DIAMNIADIO Marl– Treatment - lime-Road

Elaboration and Mechanical Characterization of Composites Reinforced with Fiber of Typha Australis

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The Typha Australis is a reed whose presence in the Senegal River valley is subject to many problems in health, fishing, etc. One way to fight against its proliferation is to take advantage of this plant by valorizing it in the field of composites as reinforcements. The objectives of this study are to extract Typha fibers and to characterize from a mechanical point of view the composites reinforced with Typha fibers. To do this, Typha plant is harvested according to the standard NS 02 – 061 [1] of Senegalese cut and these fibers extracted with a plastic comb [2] are dried in the sun for 3 days to remove all moisture [3]. The fibers are then used for reinforcements of composite in an epoxy matrix. The composite is made according to the NF-EN-527-5 type A standard [4] for long fibers. Mechanical tests are performed on these specimens at a speed of 2 mm/min according to this standard. The results show that the addition of long fiber of Typha increased the maximum tensile strength of the epoxy from 14.9 MPa to 51.4 MPa with a Young's modulus that also increased from 2.2 GPa to 5.4 GPa. Nevertheless, with these good results observed, the elongation at break of the epoxy alone equal to 0.44% is higher than the fabricated composite. It should be noted that the orientation of the fibers with respect to the applied mechanical load has a significant influence on the mechanical properties of biocomposites as explained by Nouri [5]. In view of these results, the composites reinforced of fibers of Typha Australis can be used in the field of furniture manufacturing, of automotive parts, of partition panels.

Keywords : Typha Australis, Fibers, extraction, composite,

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Combined Effect of Ground Granulated Blast-Furnace Slag and Metakaolin on the Performance of Recycled Self-Compacting Concrete

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The world is currently facing major challenges in controlling construction and demolition waste and preserving the natural environment. The recycling and reuse of concrete waste in the form of aggregates can be an effective solution to protect the environment. In this experimental research, the synergistic effect of ground granulated blast-furnace slag (GGBFS) and metakaolin (MK) on the performance of recycled self-compacting concrete (RSCC) were investigated. A total of five RSSC mixtures were produced by partially replacing cement by GGBFS and MK including control, ternary mixtures. Ternary mixtures were obtained by replacing cement by GGBFS at a constant level of 15% and MK at replacement content of 0%, 5%, 10% and 15% by weight. The water to binder ratio was kept low at 0.40; cement content and superplasticizer were maintained constant for all concrete mixtures. The evaluated rheological properties of RSCC mixtures were slump flow, V-funnel, L-Box, and the segregation resistance test. The mechanical and durability properties were also performed. The experimental results indicated that the combined use of GGBFS and MK in RSCC mixtures met the EFNARC standard requirements of filling ability, passing ability and resistance to segregation. A significantly reduction in the porosity of RSSC mixtures was observed and as a result an enhancement in compressive strength. This study also indicated that durability properties were improved. Ternary mixture with 15% GGBFS and 15% MK exhibited the best strength and durability properties to produce a sustainable recycled self compacting concrete.

Keywords: Slag (GGBFS), metakaolin, recycled self-compacting concrete, rheological properties, strength.

Condition Assessment of a Reinforced Concrete Railway Bridge Subjected to Alkali Silica Reaction (ASR) Deterioration in Johannesburg

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In the 1940's, a reinforced concrete railway bridge located in central Johannesburg was constructed using Witwatersrand Quartzite, at the time, unknown to be an alkali-silica reactive aggregate. The bridge currently displays signs of distress in the form of severe map-cracking. This study presents preliminary results of a series of tests that have been conducted to characterize the severity of ASR deterioration in the bridge. Twelve concrete cores were extracted from various locations of the railway bridge, which displayed varying degrees of visual distressed, for testing. A visual assessment was conducted globally on the entire structure as well as locally (using the damage rating index) on the extracted cores. The free alkali content was determined as well as the mechanical properties of the concrete (compressive strength and damage stiffness test). Future work will be conducted on the extracted cores to determine the residual expansion capacity of the concrete subjected to ASR



POSTER PRESENTATERS

Characterization and Fabrication Bio-sourced Brick based Lignocellulosic Plants for Low-cost Building

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Lignocellulosic plants are composite materials increasingly used for reinforcing structural and insulating element. For this, physical-chemical and thermal properties of used materials should be known. Indeed, the main objective of this present work is to produce slab bricks based on clay mixed to a natural plant so-called typha, an insulated bio-sourced and rice husk, with respect to the environment and, for low-cost construction of the Senegalese Federation of Habitant (FSH) composed mainly of women. This is a project aim is to resettle families of the FSH women who have suffered the damage caused by the floods in the suburbs of Dakar.
Indeed, physico-chemical properties of materials for a modeling of bio-sourced bricks medium-heavy slabs clay-based slabs mixed with typha fibers and rice husk, intended on the one hand for the construction of slabs and floors and on the other hand to model bio-sourced bricks light slabs used as sound and thermal insulation in buildings. Bricks are characterized to carry out the mechanical and thermal properties of the materials. Physico-chemical study of the fibers show water contents of 4.26% for the rice husk while 7.03% for large typha fibers and 7.47% for small typha fibers absorption rates up to 76.95% for rice husk; 85.18% large typha fibers while 90.83% small typha fibers. The tests carried out show that the mass of the bricks decreases according to the volume of water.

Keywords: Bio-sourced – Brick - Clay – Typha – Characterization – Low-cost – Building

Optimization and Characterization of Adobe and BTC bricks based on Raw Earth for Low-cost and Sustainable Buildings

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The present work consists of elaborating raw earth bricks used as element to realize low-cost, high quality, comfortable and durable buildings. Adobe and BTC bricks based on laterite have been devoted in numerous experimental studies. Indeed, physical characteristics of laterite soil from Sindia, a locality in sixty kilometers from Dakar, used as earth material, show the presence about 59% of gravel (2 – 20 mm) ; 37% of sand (0.02 - 2mm) and, 4% of silt and clay (0.002 - 0.02 mm). Soil contents low clay with 17.6% plasticity index a non-swelling mineralogical composition of kaolinite type and 0.51% of water with low absorption rate of 35.33% and 1308.59 kg/m^3 of bulk density. Researchers advance consider soil as one of the best suited raw earth for construction when it contains fractional clay of about 10 to 30% as result of natural binder of sand and gravel. Therefore, addition of mineral (sand, clay), vegetable (typha) and industrial (cement) could be good stabilizer. This fact improves very as well as its performance related to their thermal comfort and mechanical resistance. Actually, our results reveal that sample of 29/14/9.5 of BTC stabilized with 5% of cement and 50% of sand, for mechanical tests, an average of 1.23 MPa in agreement of standard design of BTC which should be lower than 2.4 MPa.

Keywords: BTC – Adobe – Brick – Clay – Typha – Characterization – Low-cost – Building

Physical Characterization of Excavated Soils in Diamniadio-Senegal

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The building industry is a concern in terms of health, energy consumption and environmental impacts. With more than 40% of the world's energy consumption, construction remains one of the most energy-intensive sectors and also one of the most impactful on the environment (nearly 38% of global greenhouse gas emissions in 2019). An in-depth analysis of the construction sector shows that building materials, specifically cement and iron, contribute significantly to the high cost of construction. Concrete, the most commonly used material in Senegal, is unsuited to the climatic conditions of Sahelian countries. It has poor thermal properties that offer no guarantee of thermal comfort inside buildings. In addition, cement production consumes a lot of energy and is a source of greenhouse gas emissions. Faced with environmental and energy concerns, the choice of adequate materials is crucial in order to limit the environmental impact and to ensure a healthy and comfortable interior environment. Thus, research on the use of local clay resources for the production of mud bricks is underway. However, the use of swelling clays is at the origin of important problems in construction. Indeed, because of the phenomena of shrinkage-swelling of these clays, many pathologies at the level of the foundations of the houses located in certain zones are to be noted. Thus, for a good prediction of the mechanical and thermal behavior of a material, in particular According to the hygrometry, it is important to determine its physical properties. This is why our study focuses on the physical characterization of the excavated soils of Diamniadio. We were mainly interested in the determination of organic matter content, natural water content, apparent and absolute density, Atterberg limits, and particle size. The results show that our material has a bulk density of 1610 kg/m^3, an organic content of 1.7 % and a plasticity index of 20 % which shows that it is a non-organic and plastic material.

Keywords: excavated soils of Diamniadio, organic matter content, natural water content, apparent and absolute density, Atterberg limits, particle size analysis.

Influence of Grain Size on the Surface Heave Due to Sodium Chloride Internal Crystallization Induced by Evaporation in a Granular Material

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Crystallization of a salt in a porous medium can lead to the generation of stresses on the pore wall. This stress generation mechanism causes the phenomenon of surface heave, i.e. the upward displacement of the porous material surface. This surface heave phenomenon is studied from experiments with random packings of particles (glass beads) confined in a quasi-2D cell when the crystallization of sodium chloride is induced by evaporation. It is shown that the grain size has a significant impact on the surface heave. The experiments reveal the existence of an optimal grain size maximizing the heave. For our experimental conditions, the analysis of the experiments suggest that the bead size dependence is not related to the mechanical aspect of the problem but is rather linked to the impact of the bead size on the morphology and internal properties of the growing subflorescence.

Keywords: Salt damage, porous medium, surface heave, subflorescence, durability

Influence of Clay and Fines Content on Bending and Tensile Strength of Alkaline Phenolic Molds in a Foundry Operation.

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Moulding is an essential process in metal casting. It is important that the moulds have adequate strength in order to be able to withstand the weight from the poured molten metal. There is several sand characteristics that influence the binding properties of the alkaline phenolic binder to the silica sand grains. This therefore affects the mould strength development. The clay content and fines are some of the properties that can influence the mould strength development. The aim of this research was to find out if the influence on different types of strength is the same or it could differ dependent on which strength is been measured on a particular strength. Data was collected in a foundry over a period. The data was from sand tests on raw silica sand for clay content and fines and mixed sand from the mixer for bending and tensile strength. Every batch was tested concurrently for the above-mentioned properties from the mixer. The results showed that the different characteristics influence the different types of strength differently. This therefore means you cannot generalise the influence of sand properties on mould strength, different types of strength can be influenced differently by different sand characteristics either positively or negatively.

Physical and Thermal Characterization of Class Powder and Coffee Grounds for the Elaboration Construction Materials

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Concrete is generally the most used building and construction material. Its production requires a large amount of cement, releasing approximatively one ton of CO_2 to the atmosphere for every ton of cement [1]. However, the use of glass and coffee grounds in concrete could be an ecological and economical alternative as a new source of building and construction materials. The objective of this work is to determine the physical and thermal proprieties of class powder and coffee grounds.
Experimental studies with the helium Pycnometer and the Mould method were used to determine the absolute density and bulk density respectively. These results showed that the values found for the different kinds of glass follow the same trends. Thus, for coffee grounds, they showed a difference. In addition, the analysis of the particle size curves made it possible to calculate the fineness modules. These results showed that coffee grounds can be classified as a fine material, while glass is mainly composed of coarse elements. The box method is used to measure thermal conductivity. The obtained results showed that the samples studied can be considered as thermal insulators with respectively 0.086 W/m.K for coffee grounds and 0.09 to 0.10 W/m.K for glass wastes.
Indeed, these results can be compared with those found in the literature. For example, Mageswari and Vidivelli showed that glass powder has a density of 1310 kg/m^3 [2]. According to Premalatha and Srinivasan, glass has a fineness modulus of 3.16 [3]. On the other hand, Francky indicates that coffee grounds have an absolute and apparent density of 1160 and 430 Kg/m^3 [4]. Hanif and al, state that coffee grounds have a density of less than 1900 kg/m3 [5]. The results of the physical and thermal characterization will be useful for the development of building and construction materials based on glass powder and coffee grounds.

Keywords: Coffee, glass, density, fineness modulus

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SYMPOSIUM-02
MATERIALS FOR **AGRICULTURE**



KEYNOTE
SPEAKERS



Tahir Abdoulaye DIOP *is a Senegalese citizen and an Emeritus Professor of Universities. He holds a Master of Science in Natural Sciences in 1987 from the University of Dakar in Senegal, a Master of Science in Forest Science in 1990 from the Laval University of Quebec in Canada, and a Ph.D. degree in Plant Biology and Physiology in 1995 from the University of Angers in France.*

Professor DIOP is currently the Director of High School of Agricultural Sciences and Food and also in charge of Research and Innovation at the University Amadou Mahtar MBOW (UAM) of Dakar. In this capacity, he coordinated the development of training models for schools dedicated to agriculture and scientific research.

Professor DIOP's research areas are focused on fungal biotechnologies, plant microorganism interactions for sustainable agriculture.

In terms of research, Mr. DIOP is founding Director of the Laboratory of Fungal Biotechnologies of Cheikh Anta DIOP University (UCAD) in Dakar and has developed a rich partnership at national and international level for research and training.

Mr. DIOP has supervised several Master and PhD students and published more than 100 scientific articles. He is currently a member of the steering committee of the Doctoral School of Life Sciences, Environment and Health of Dakar university and also the National System of Agrosylvopastoral Research of Senegal.

Administratively and at the national level, Mr. Diop was Technical Advisor and Director of Research at the Ministry of Higher Education and Research of Senegal from 2005 to 2012.

Promoting Fungi for Sustainable Agriculture in Africa

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The soil hosts fungi with a varied biotrophy and very cosmopolitan. A good exploitation of fungal biotechnology is a promising way to achieve food security in Africa. These fungi improve soil structure, regulate hydromineral nutrition, plant growth and resistance to certain diseases.
Different research topics related to ecophyqiology, biology and domestication of symbiolic, associated and edible fungi have been carried out in our laboratories This presentation first relates the point of the current state of research carried out on the cultivation and then identifies the prospects the use of fungal biotechnologies for a sustainable and competitive agriculture.



*Since 2020, **Dr. Christian Dimkpa** has been the Chief Scientist and Head of the Department of Analytical Chemistry at the Connecticut Agricultural Experiment Station (CAES) based in New Haven, Connecticut (CT), United States. At CAES, Christian conducts dual functions in research and regulatory activities. His research interests include understanding elemental (including toxic metals) implications in the agriculture-food-environment continuum and designing strategies to leverage elements' role as nutrients for enhancing crop production. To that end, he conducts active research on nanotechnology applications and implications in agriculture and the environment with a focus on phosphorus, nitrogen, copper, zinc, and silver. Christian explores the use of biomaterials to improve the plant use efficiency of nutrient elements. In his regulatory role, Christian oversees a group of scientists and technicians involved in detecting, quantifying, and reporting toxic elements, pesticides, mycotoxins, polychlorinated biphenyls, and other contaminants in human food, animal feed, soil, and environmental samples, in response to needs by CT State regulatory agencies. Prior, Christian was a Development Scientist at the International Fertilizer Development Center in Muscle Shoals, Alabama, USA (2014-2020), and a Research Assistant Professor in the Biology Department of Utah State University, Logan, Utah (2009-2014). Christian Obtained his PhD in Bioenvironmental Sciences in 2009 from the University of Jena, Germany, under the auspices of the International Research School of the Max Planck Institute for Chemical Ecology.*

Nutrient Management for Sustainable Development: A Case for Chitosan

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Agricultural production in Africa must increase by some 120% if the continent must sustainably feed its growing population by 2050. To achieve food self-sufficiency while preventing further damage to ecosystems, such increase must come from intensification of agricultural production, rather than from extensification via increasing the land hectarage under cultivation. Agrochemicals such as fertilizers are critical inputs for agricultural intensification. Unfortunately, fertilizers are applied at 15% of recommended rates in Africa, which, when combined with the inherent low use efficiency (<30%) of conventional fertilizers, results in crop yield gaps in the continent, relative to other regions of the world. In particular, phosphorus (P), abundantly available in Africa, suffers from high insolubility in its raw (rock phosphate) form, and from high leaching and run-off losses in the processed water-soluble fertilizer-grade forms. This is even as the long-term sustainability of global P resources remains questionable. Accordingly, strategies are required involving harnessing the huge African natural resources to improve plant use efficiency of agrochemicals such as P. Notably, use of biogenic polymers from biowaste to modulate nutrient availability to maximize fertilize use efficiency and increase crop yield is gaining momentum elsewhere but in Africa. Chitosan, an amino-polysaccharide-based polymer is a renewable and environmentally-friendly material produced from seafood waste. High biodegradability, biocompatibility, and non-toxicity are key features lending chitosan to applications in agriculture. Given the huge presence of both inland and continental water resources, African countries are in a good stead to harness their aquatic resources for the development of chitosan-based agrochemicals. This presentation describes ongoing research on the use of nano-scale chitosan and an unusual P source, tripolyphosphate, for the formulation of P fertilizers with modulated P solubility and leaching loss. The potential for use of the formulation in increasing P uptake by plants and engendering overall agronomic benefits are discussed.

Keywords: Phosphorus; nutrient use efficiency; nanotechnology; nano-chitosan; biopolymer.



Biosketch: *Dr. Santra is a Professor at the University of Central Florida holding a joint appointment with the NanoScience Technology Center and the Department of Chemistry. He is the founding director of UCF Materials Innovation for Sustainable Agriculture (MISA) Center. He has been actively working in the field of Nanoscience and Nanotechnology for over 20 years focusing on nanoagriculture and nanomedicine areas. He has published 93 peer-reviewed research articles, 7 review articles, 11 book chapters and delivered 96 invited talks. He has been awarded 34 patents including 26 US patents. His research has been funded by National Science Foundation, United States Department of Agriculture, Citrus Research and Development Foundation, California Department of Food and Agriculture, Environmental Research and Education Foundation and several industries with a portfolio of over $6.0 Million research funding.*

Crop Protection with Nanotechnology-Enabled Formulation

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To achieve global food security, it is essential to develop a roadmap that would lead to sustainability in agrochemical input. With emerging threats of global climate change and politicalunrest, there is an unprecedented demand for improving agrochemical use-efficiency through innovation. Nanotechnology is a platform that demonstrated strong promise in recent years in proving robust tools to improve crop production practices at reduced agrochemical load. Academicand industry initiated innovative research in past two decades have led to significant advancementin this area, resulting in introduction of new nano-enabled agrochemicals such as nanofertilizers to the market place. Although extensive research is underway, due to stringent regulatory restrictions, nanopesticides will likely take much longer to penetrate the pesticide market. Excessive use of conventional crop protection chemicals has increased risks of development of pathogen resistance. For example, copper (Cu) bactericides/fungicides are widely used in the agriculture industry in the U.S and worldwide on many crops. There is an increasing concern of Cu accumulation in field soil, Cu leaching potential into the surrounding ecosystem and development of bacterial resistance. However, using nanotechnology it is possible to reduce Cu load per application or develop suitable Cu alternatives (such as Mg and Zn). This presentation will focus on laboratory, greenhouse and field experiments to demonstrate the efficacy of severalmetal-based crop protection nanoformulations, along with the challenges associated with developing industrially viable formulations and approaches to minimize regulatory challenges.

Keywords: Nanotechnology, copper, zinc, magnesium, bactericide, fungicide, citrus canker, huanglongbing, pierce's disease, bacterial spot



INVITED SPEAKERS

Using Physiological and Molecular Markers to Select Drought Tolerant Cowpea Mutant Lines Obtained by Gamma Irradiation

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Cowpea is one of the most important crop legume grown in tropical and subtropical regions of Africa, Latin America and Asia, South of Europe and Southern of Northern America for its use in human consumption and animal feeding. Despite this importance, the production of the crop is hampered by a wide range of constraints including biotic and abiotic factors such as drought raising the need to implement a relevant breeding program. The objective of this study was to select new cowpea mutant lines tolerant to drought for increasing cowpea production.
For this purpose, healthy seeds of two cowpea varieties namely Ndout and Bambey 21 as well as the mutant UCAD 2 were divided in three batches for each genotypes then irradiated with three doses 200 Gy, 300 Gy and 400 Gy, respectively using a cobalt 60 source Gammacell (Model No. 220). Mutant populations were developed until to the 7th generation (M7) that were sown using pedigree methods. The plants of 20 days old were subjected to drought during 38 consecutive days then, relative water content, chlorophyll content, biochemical markers (proline, catalase, ascorbate peroxidase, MDA and SOD) were analyzed.
Our results revealed one (1) mutant line of Ndout that showed stay green character. This line did not show significant variation in relative water content, in proline and MDA content, but its chlorophyll a, b and chlorophyll total contents increased in drought conditions regardless the gamma irradiation dose. The analysis of the biochemical markers showed an increase of ascorbate peroxidase (APX) and catalase activities, no variation for superoxide dismutase activities under drought stress. APX activity was positively correlated with chlorophyll a (0.44), chlorophyll b (0.46), total chlorophyll (0.48) and negatively correlated with MDA (-0.43). Based on physiological and biochemical markers, principal component analysis revealed 4 main groups. Our studies suggested that the stay green mutant line can be used in a breeding program.

Keywords: Cowpea; *Vigna unguiculata*; molecular breeding; gamma irradiation; mutants

Assessment of Yield-Related Traits in a Population of Recombinant Inbred Lines of Peanut (*Arachis Hypogaea* L) Developed for High Oleic Content

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Peanut (*Arachis hypogaea* L.) is the most important cash crop in Senegal. Recently, peanut'exports from Senegal have gained a significant increase with international demand of Spanish-type varieties. However, still now all released varieties are low oleic acid content and that is hindering peanut industry development in Senegal. In order to provide farmers with high oleic peanut varieties we have developed a population derived from a cross between Turquie and Schubert. Turquie is a Virginia-type peanut variety with big seed size while Schubert is a Spanish-type bunch variety with earliness and high oleic content. We evaluated recombinant inbred lines along with 10 varieties as checks among which the parental lines for yield related traits at Nioro Research Station (Senegal) using an augmented design. After harvest, pod weight (PW) per plant, total kernel weight (TKW) per plant, sound kernel weight (SMK) per plant and 100 seed weight (HSW) were evaluated.
Analysis of variance revealed significant effect of the genotypes for all traits except pod weight. In addition, significant differences among families were observed, indicating large genetic and phenotypic variability in that population. Among tested families, eight have TKW significantly higher than that of the parental line Schubert. And five lines have HSW higher than 65 g. These are promising lines that would be released as high oleic peanut varieties with better seed quality traits.

Keywords: Peanut, oleic acid, recombinant inbred lines population, yields-related traits, seed quality traits.

Salt Tolerance in Glaberrima rice: Mechanism and approach using proton induced x-ray emission

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Salt tolerance is an important constrain for Africa rice. Soil salinity is one of the major constraints affecting rice production worldwide, especially in the northern part of Senegal. Susceptibility or tolerance of rice plants to high salinity is a coordinated action of multiple stress responsive genes, which also interacts with other components of stress signal transduction pathways. Salt tolerant varieties can be produced by using two different sets of germplasm. One comprised of a diversity panel of 317 accessions of O. Glaberrima received from Africa Rice Genetic Resources Unit and checks: FL478 (salt tolerance), IR 29 (salt sensitive), Sahel 210 and Sahel 134. The second is comprised of an indica diversity panel of 330 genotypes received from IRRI. Both sets were evaluated under control conditions where they were grown under irrigated lowland conditions using non-saline river water (EC <1 dSm-1) and also under saline conditions in a concrete-lined field where salinity was maintained at 4 dSm-1. In this review, we have updated on mechanisms and genes which can help in transferring of the salt tolerance into high-yielding rice varieties. We have focused on the need for integrating plant biology into transgenic and breeding approaches to develop high-yielding as well as salt tolerant rice varieties. PIXE studies have been performed for determination of different elements in rice plants. The micro beam analytical technique existent at the iThemba LABS was applied for the 2D image mapping of fresh rice tissues. The technique will be used to measure the concentration of low atomic mass elements based on the targeted it in the rice plants with detection limits of typically 1-10µg/g.



ORAL
PRESENTATERS

Decarbonation Reaction from $NaHCO_3$ for CO_2 Production

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CO_2 can be produced by thermochemical conversion of bioresources or from the removal of carbonates from soil or water or by acid-base reaction. The most decarbonation reaction used is between sodium bicarbonate ($NaHCO_3$) and an acid product. During this reaction, protons (H^+) of the acid react with $NaHCO_3$ to produce CO_2, H_2O and ions. In the literature, it has been shown CO_2 releasing can occur during water treatment [1], food industry [2] or medicine [3].
The aim of this study is to produce CO_2 from an acid-base reaction between sodium bicarbonate ($NaHCO_3$) and acid phosphates. The influence of operating parameters such as stirring speed, quantity of acid and basic compound, particle size of the solids has been studied. Results showed the impact on the decarbonation rate and the quantity of CO_2 release as a function of the experimental parameters. From experimental results, kinetics of decarbonation were determined to identify the rate bit also the order of the reaction as a function of the phosphate used. The particle size of the solid reagents is an important parameter influencing the decarbonation reaction due to the shrinking core process which is determining during an acid attack. These results help to optimize the CO_2 production as a function of the physico-chemical properties of the reagents.

Keywords: Decarbonation, Kinetics, Physicochemical parameters, Rate of reaction, CO_2

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Biodegradable Solid Lubricant

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Design of solid lubricants has largely been based on phase change or interlayer slippage. The former is incompatible with granular flow especially in heavy machinery while the later, like talc, are often toxic to the users and to the environment. Use of solid lubricants in agriculture, however, requires the material be affordable, biodegradable, and safe to the farmer and the environment. This talk described a surface chemistry-based approach to design of medium and high lubricity solid lubricants. We create amphiphobic surfaces on a fibrous material through surface-water driven oligomerization. The amphibocity enables tolerance of high humidity allowing the material to function as a seed lubricant at elevated humidity. We extend this work to design of graphitic tubes that show enhanced lubricity albeit with decreased humidity tolerance. Enhancing defects in this graphitic material improves high humidity performance. Underlying chemistry and tribological performance will be discussed.

Keywords: Biodegradable, Solid Lubricant, Agriculture, Solid lubricant, Surface chemistry

Effect of the Combination Deficit Irrigation-Biochar on Tomato Yield, Growth, and Irrigation Water Use Efficiency in a Sandy Clay Soil, in the Context of Climate Change in Senegal

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In Senegal, the long period of dry season, the insufficient amount of water in the rainy season, the water pollution, and the increase of population, led to a decrease of freshwater resources and put it under pressure and competition among the users. Inadequate agricultural water management combine with weak capacity of most Senegalese soils to hold water will led to more inefficient use of irrigation water. This study aims to assess the impact of biochar on tomato yield, growth, and on irrigation water use efficiency (IWUE) in a sandy-clay soil in West Africa-Senegal. A one season factorial experiment was conducted with combination deficit irrigation-biochar from February 2021 to June 2021 with three irrigation level i.e full irrigation (recommended-W0 = 40 L/day), 75% of full irrigation (W1 = 30 L/day), and 50% of full irrigation (W2 = 20 L/day), and three amount of biochar i.e 3 kg/m^2 (B2), 50%B2 (B1= 1.5 kg/m^2), and 0%B2 (B0 = 0kg/m^2) (control). The measurement of different parameters started 10 days after transplantation. The reduced irrigation –biochar did not influence all the growth parameters of the tomato. W0B1 showed greatest total grain yield 20.62t/ha, against 17.76t/ha for W0B2, 13.45t/ha for W0B0, and 12.12t/ha for W1B2. In contrary the treatment W2B2 recorded the lowest yield. W0B1 (1845.76 kg m^{-3}), W0B2 (1521.63 kg m^{-3}), and W0B0 (1441.56 kg m^{-3}), respectively, obtained the greatest IWUE. But W0B0 and W0B2 did not show significant difference with W1B2 (1320.33 kg m^{-3}). The results suggest that in the area of insufficient water availability, biochar at the rate of 3g/m^2 (30t/ha) gives an optimum production of tomato. But W1B2 is more water saving and do not significantly affect the yield of tomato in a Sandy Clay soil. When water is sufficient, it is preferable to use a moderate amount of biochar (B1=1.5g/m^2) for efficient water management. Biochar regulates the water fluxes into the soil.

Keywords: Biochar; Deficit-Irrigation; Water use efficiency; Plant yields; Sandy-Clay soil



POSTERS
PRESENTATERS

Partial Purification and Characterization of Phytocystatin from *Calotropis procera* with Antibacterial Activities

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Phytocystatins are large family of plant bioactive protein inhibitors of papain-like cysteine proteases. In this study, we present the partial purification of phytocystatin isolated from *Calotropis procera* latex. The Phosphate buffer extract from the latex of *C.procera* with papain inhibitory activity was concentrated by cold acetone precipitation and was further subjected to purification using ammonium sulphate fractionation and Hydrophobic chromatography on Phenyl sepharose column. Cold acetone precipitated extract gave 9.6% protein yield with 63% inhibition of protease. An estimated molecular weight of 18 kDa was obtained on sodium dodecyl sulphate (SDS) polyacrylamide gel electrophoresis and optimum temperature and pH at 60^0C and 6.0 respectively. The fifty percent inhibitory concentration (IC_{50}) of the inhibitor on Papain enzyme was 23.10±1.2 µg/ml with inhibitor binding constant (Ki) of 8.0µg/ml, suggested high affinity between inhibitors and enzymes. Chemical modification of some key amino acids presents in the binding site of the partially purified phytocystatin, revealed the presence Cysteine and Histidine. More interestingly, phytocystatin presents a strong antimicrobial activity against human pathogens such as *Staphylococcus aureus* and *Enterococcus faecalis*, which is a new property for this family of protease inhibitors. These results highlight the biotechnological potential of phytocystatin from latex of this plant.

Keywords: *Calotropis procera*; plant protease inhibitor; phytocystatin; papain inhibitor; antibacterial;



SYMPOSIUM-03
MATERIALS FOR **ENERGY**



KEYNOTE SPEAKERS



Prof. Dr. Lionel Vayssieres

French, born in North Africa in 1968, Lionel obtained a High School degree in Mathematics & Life Sciences in 1986 in Valence, France. Thereafter, he moved to Paris and obtained a 2-year degree in Natural Sciences & Biophysics in 1988, a BSc in 1989 and a MSc in 1990 in Physical Chemistry, an advanced degree in Inorganic Chemistry in 1991 and a PhD in Chemistry in 1995 (after his 1994 military duty as a scientist for the French Navy) from the Université Pierre et Marie Curie, Paris, France for his research work on the Interfacial & thermodynamic growth control of metal oxide nanoparticles in aqueous solutions. Thereafter, he joined Uppsala University, Sweden in early 1996 as a postdoctoral researcher for the Swedish Materials Consortium on Clusters & Ultrafine Particles to extend his concepts and develop purpose-built oxide nanomaterials by aqueous chemical growth such as highly oriented nanorod-arrays for photoelectrochemical applications and to characterize their electronic structure by x-ray spectroscopies at synchrotron radiation facilities. Thereafter, he was invited as a visiting scientist at: the University of Texas at Austin, Chemical Engineering Department and Texas Materials Institute, USA; the UNESCO Centre for Macromolecules & Materials, Stellenbosch University, and iThemba LABS, South Africa; the Glenn T. Seaborg Center, Chemical Sciences Division and the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory (LBNL), CA, USA; The Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland; the University of Queensland, Australia; Karlsruhe Institute of Technology (KIT), Germany; Nanyang Technological University (NTU), Singapore and the Brazilian Nanotechnology National Laboratory (LNNANO) in Campinas, Brazil. He was also an Independent Scientist at the National Institute for Materials Science (NIMS) in Tsukuba, Japan for 8 years (2004-2012). He has (co-)authored 100+ publications in major international journals, proceedings, books and book series which have generated 15000+ citations since the year 2000. He has given 425 talks in 33 countries including the prestigious Spring MRS Symposium X lecture in 2015. He also acted as an organizer, chairman, executive program committee, and advisory member for major international conferences and projects worldwide as well as an Expert member for numerous funding agencies and scientific prizes worldwide. He is also, since 2003, the founding Editor-in-Chief of the International Journal of Nanotechnology and a referee for 100+ SCI journals. Since 2012, he is a full-time High-Talent research professor, chief scientist, co-founder and scientific director of IRCRE-International Research Center for Renewable Energy (810+ publications including 780+ research articles published in 205+ different journals of average 2021 Impact Factor = 8.9 and 35000+ citations), School of Energy & Power Engineering at Xi'an Jiaotong University, China. He's the recipient of the 2014 Sanqin Provincial and the 2016 National Chinese Government Friendship Awards, one of the Most Cited Researcher in China in the field of Materials Science & Engineering for 2014-2021 (Scopus/Elsevier) as well as one of the 2016 American Ceramic Society Global Ambassador Awardee. He is ranked in the 2021 Top 2% World Scientists Ranking (Stanford Univ. study) as #174 among 89177 scientists (Top 0.19%) in Nanoscience & Nanotechnology.

A Place in the Sun for Artificial Photosynthesis and Green Hydrogen Generation

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Undoubtedly, this decade is experiencing the widest consequences of man-made activities with environmental disasters at a record high. Staggering air/water pollution and catastrophic drought and flooding worldwide represents the most important problem humanity and the environment facing. It is now critical to transition to new sustainable societies where environmental, energy, and economic policies are no longer based on endless-growth financial models and fossil fuel technologies to rapidly and substantially decrease our environmental footprint and health impacts.

The transition to hydrogen-based energy and economy is ideal to reach carbon-zero societies. However, most of the hydrogen produced still comes from nonrenewable sources which produces large amount of carbon dioxide. The most natural, cleanest and sustainable way to produce hydrogen at large scale is by solar seawater splitting.

Our strategy is to use easily scalable, clean, and cost-effective fabrication techniques based on highly efficient materials made of earth-abundant elements, easily extractable and recyclable rather than expensive, scarce, and toxic ones to fabricate devices consisting of oriented arrays of quantum rods/dots of high purity synthesized by aqueous chemical growth at low temperature without surfactant and with controlled dimensionalities, engineered surface chemistry, intermediate bands for high sunlight conversion, bandgap and band edges optimized for long-term stability against photocorrosion, operating conditions at low/no bias without sacrificial agent in pure and simulated (sea)water. Such engineered characteristics, combined with in-depth investigation of size-dependent and interfacial electronic structure, electrical and photoelectrochemical properties provide better fundamental understanding and structure-efficiency relationships for a cost-effective and sustainable generation of *green* hydrogen from the two most abundant and geographically-balanced free natural resources readily available at the surface of our blue planet, that is the sun and seawater.

An overview of the past decades of pioneering research as well as the latest advances in solar water splitting for green hydrogen generation will be presented.

Keywords: Water splitting, Solar fuel, Nanotechnology, Electronic structure, Aqueous synthesis



Federico Rosei *(MSc (1996) and PhD (2001) from the University of Rome "La Sapienza") is Full Professor at the Centre Énergie, Matériaux et Télécommunications, Institut National de la Recherche Scientifique, Varennes (QC) Canada, where he served as Director (07/2011–03/2019). He held the Canada Research Chair (Junior) in Nanostructured Organic and Inorganic Materials (2003–2013) and since May 2016 he holds the Canada Research Chair (Senior) in Nanostructured Materials. Since January 2014 he holds the UNESCO Chair in Materials and Technologies for Energy Conversion, Saving and Storage. Dr. Rosei's research interests focus on structure/property relationships in nanomaterials and their use as building blocks in emerging technologies. His research has been supported by multiple funding sources from the Province of Quebec, the Federal Government of Canada as well as international agencies, for a total in excess of M$ 18. He has worked in partnership with over twenty Canadian R&D companies. He is co-inventor of three patents and has published over 435 articles in prestigious international journals (including Science, Nature Photonics, Proc. Nat. Acad. Sci., Adv. Mater., Angew. Chem., J. Am. Chem. Soc., Adv. Func. Mater., Adv. En. Mat., Nanolett., ACS Nano, Biomaterials, Small, Phys. Rev. Lett., Nanoscale, Chem. Comm., Appl. Phys. Lett., Phys. Rev. B, etc.), has been invited to speak at over 340 international conferences and has given over 255 seminars and colloquia, over 60 professional development lectures and 45 public lectures in 49 countries on all inhabited continents. His publications have been cited over 20,800 times and his H index is 76. He is Fellow of numerous prestigious national and international societies and academies, including: the Royal Society of Canada, the European Academy of Science, the Academia Europaea, the European Academy of Sciences and Arts, the African Academy of Sciences, the World Academy of Art and Science, the World Academy of Ceramics, the American Physical Society, AAAS, the American Ceramic Society, the Optical Society of America, SPIE, the Canadian Academy of Engineering, ASM International, the Royal Society of Chemistry (UK), the Institute of Physics, the Institution of Engineering and Technology, the Institute of Materials, Metallurgy and Mining, the Engineering Institute of Canada, the Australian Institute of Physics, Honorary Fellow of the Chinese Chemical Society, Foreign Member of the Mexican Academy of Engineering, Foreign Member of the Bangladesh Academy of Sciences, Senior Member of IEEE, Alumnus of the Global Young Academy and Member of the Sigma Xi Society. He has received several awards and honours, including the FQRNT Strategic Professorship (2002–2007), the Tan Chin Tuan visiting Fellowship (NTU 2008), the Senior Gledden Visiting Fellowship (UWA 2009), Professor at Large at UWA (2010–2012), a Marie Curie Post-Doctoral Fellowship (2001), a junior Canada Research Chair (2003–2013), a senior Canada Research Chair (2016–2023) a F.W. Bessel Award (Humboldt foundation 2011), the Rutherford Memorial Medal in Chemistry (Royal Society of Canada 2011), the Herzberg Medal (Canadian Association of Physics 2013), the Brian Ives Lectureship (ASM international 2013), the Award for Excellence in Materials Chemistry (Canadian Society for Chemistry 2014), the NSERC EWR Steacie Memorial Fellowship (2014), the José Vasconcelos Award for Education (World Cultural Council 2014), the IEEE Distinguished Lectureships (NTC 2015–2016 and Photonics Society 2020–2022), the Lash Miller Award (ECS 2015), the Chang Jiang Scholar Award (China), the Khwarizmi International Award (Iran), the Recognition for Excellence in Mentorship (American Vacuum Society 2015), the Selby Fellowship (Australian Academy of Sciences 2016), the J.C. Polanyi Award (Canadian Society for Chemistry 2016), the Outstanding Engineer Award (IEEE Canada 2017), the President's Visiting Fellowship for Distinguished Scientists (Chinese Academy of Sciences 2017), the Sigma Xi Distinguished Lectureship (2018–2020), the Sichuan 1000 talent (short term) award, the Lee Hsun Lecture Award (2018), the Changbai Mountain Friendship Award (2018), the IEEE Montreal Gold Medal (2018), the APS John Wheatley Award (2019), the Blaise Pascal Medal (European Academy of Science 2019), the Guangxi Golden Silkball Friendship Award (2020), the TMS Brimacombe Medal (2021), the Wolfson Fellowship (Royal Society), the Prix Urgel Archambault (ACFAS 2021), the Prix du Quebec "Marie Victorin" (2021), the J.C. Smith Medal (Engineering Institute of Canada 2022) and the Premio Nazionale "Gentile da Fabriano" (Associazione Premio Gentile, Italy 2022).*

Multifunctional Materials for Emerging Technologies

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This presentation focuses on structure property/relationships in advanced materials, emphasizing multifunctional systems that exhibit multiple functionalities. Such systems are then used as building blocks for the fabrication of various emerging technologies. In particular, nanostructured materials synthesized via the bottom–up approach presents an opportunity for future generation low-cost manufacturing of devices [1]. We focus in particular on recent developments in solar technologies that aim to address the energy challenge, including third generation photovoltaics, solar hydrogen production, luminescent solar concentrators and other optoelectronic devices [2-40].

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Turning Air and Water in to Ammonia Using Versatile Materials

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The electrochemical nitrogen reduction reaction (NRR) is an attractive alternative to minimizing the energy and greenhouse gas footprint from the current ammonia (NH_3) production process. Most NRR catalysts operate through utilizing an associative or dissociative mechanism, during which the NRR competes with the hydrogen evolution reaction (HER), resulting in low selectivity. In this presentation, we report on a new active catalyst for NRR that operates through the Mars-van Krevelen (MvK) mechanism to increase the selectivity of NRR towards NH3. This new catalyst, two-dimensional (2D) Ti2N nitride MXene, was synthesized via an oxygen-assisted molten salt fluoride etching technique. We confirmed its phase purity and stability in aqueous electrolytes using various characterization techniques, including Raman, X-ray diffraction, and UV-Vis. The Ti2N nitride MXene catalyst achieved a high Faradaic efficiency (FE) of 19.85% towards NH3 at an applied potential of –250 mV vs. RHE with a yield of 11.33 µg/cm2/hr in a 0.1 M hydrochloric acid (HCl) N2-saturated electrolyte. Further electrochemical characterizations in an Ar-saturated electrolyte suggest that the new catalyst operates through an MvK mechanism. These results can be expanded to a broad class of systems enabling the MvK mechanism and constitute the foundation of NRR technology based on MXenes.

Keywords: Sustainability, Ammonia, 2D Materials, Energy, Electrochemistry



EARLY CAREERS- SPEAKERS



Ndeye Fatou Sylla *is a postdoctoral researcher in the department of inorganic chemistry at the Dresden University of Technology, Germany. She earned both B.S and M.S degrees in Physics department at the University Cheikh Anta Diop of Dakar, Senegal. Dr. Sylla received her Ph.D. in physics from the University of Pretoria, South Africa under Prof N. Manyala and Prof B. D. Ngom in 2020. Her work was focused on activated carbon from peanut shell waste and its molybdenum-based nanocomposites for supercapacitor applications. Her doctoral work received many recognitions including National Research Foundation (NRF) and University of Pretoria postdoctoral fellowship, TWAS Research grant and visiting research fellowship at Pennsylvania and Drexel Universities, USA. Her research interest is on the development of novel porous carbon materials-based composites and their application in energy storage such as supercapacitors and Li-S battery. Currently, she is an Alexander von Humboldt-Stiftung fellow, member of OWSD, TWAS.*

Enhanced electrochemical performance of activated carbons derived from peanut shell waste

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In this work, peanut shell waste activated carbons and its composites were explored as potential electrode materials for supercapacitor applications. This study reports the enhancement of electrochemical performance of the peanut shell waste activated carbons (PAC) through (i) a pre-carbonization followed by and chemical activation (PAC), (ii) heteroatom-doping with nitrogen (NPAC). Their physicochemical, surface and electrochemical properties have been successfully achieved using various techniques. All activated carbon materials were synthesized using chemical vapour deposition (CVD) and characterized by N_2 adsorption-desorption, X-ray diffraction (XRD), Raman spectroscopy, scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), high-resolution transmission electron microscopy (HR-TEM) and X-ray photoelectron spectroscopy (XPS). The textural properties obtained were depicted with relatively high specific surface area values of 2547 $m^2\ g^{-1}$ and 1442 $m^2\ g^{-1}$ for the PAC and NPAC samples, respectively.
The electrochemical performance of the as-synthesized PAC and its composites electrodes materials have been tested in symmetric devices in 2.5 M KNO_3 aqueous electrolyte. The activated carbon-based electrodes exhibited a good electrochemical energy storage capability with a wide cell potential in the range of 1.8 - 2V. The as-fabricated symmetric supercapacitors exhibit remarkable specific energy ranging from 25 W h kg^{-1} to 35 W h kg^{-1} as a function of specific power from 900 W kg^{-1} to 1000 W kg^{-1} at a specific current of 1 A g^{-1}. Moreover, long term device stability was exhibited with an 99.8% coulombic efficiency, 83% capacity retention over a 20 000 charge/ discharge cycles and also a good rate capability after 180 h of floating at 5 A g^{-1}.



George Bepete *is an Assistant Research Professor in the Physics Department and the Center for 2-Dimensional and Layered Materials at the Pennsylvania State University. He completed his Ph.D. in Materials Chemistry at University of the Witwatersrand, Johannesburg in South Africa (2014). His thesis focused on the control of nitrogen and boron incorporation during CVD growth of nitrogen and boron doped carbon nanotubes and graphene materials. From there he joined the National Centre for Scientific Research, CNRS, in Bordeaux France, as a Postdoctoral Fellow, where he developed methods to produce surfactant-free dispersions of monolayer graphene and individualized SWNTs in water. In 2017 he received the French Carbon Society Young Researcher Award recognizing significant contributions to carbon science for his work at CNRS on surfactant-free dispersions of single-layer graphene in water. At Penn state his research is focused on the synthesis and properties of alkali metal intercalation compounds of inorganic layered materials such as hBN and their exfoliation into single layers. He is developing structure controllable methods of assembling bulk 2D-material layered heterostructures for application in energy storage and optoelectronics.*

Chemical Intercalation as a Versatile Technique for Property Tuning and Production of Layered Materials

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Introducing alkali metal atoms between the carbon layers of graphite to form graphite intercalation compounds (GICs), can tune the interlayer spacing and charge the graphite host through a variety of electronic ground states.[1] Hexagonal boron nitride (hBN) is another prototypical layered material and possesses a hexagonal network consisting of B and N atoms. Because of its structural similarity to graphite, there has been several theoretical calculations predicting host-guest redox-driven hBN intercalation compounds.[2] Based on the analogy with GICs, the hybrid structure of hBN and alkali metal atoms that are intercalated into the interlayer spacing may also exhibit interesting electronic properties and utility as a raw material for 2D materials with unprecedented physicochemical properties.[3] However, the intercalation of alkali metal in hBN has proven to be considerably more difficult than graphite. Here, we will present our latest experimental data, showing that potassium metal can be intercalated into hBN layers.[4] The K-intercalated hBN material exhibits unprecedented electronic and energy storage properties. We will also show new data on the processing and characterization of a new form of 1-dimensional sp^3 carbon called carbon nanothreads.[5]

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One-pot Hydrothermal Synthesis of Nitrogen-Doped Reduced Graphene Oxide/Hausmannite Manganese Oxide for Supercapacitor Applications

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Electrochemical energy storage (EES) devices have emerged as key components to support renewable energy sources required to mitigate the detrimental impacts brought by the use of fossil fuels and also the advanced energy demand arising from the rapid technological growth.[1] Supercapacitors (SCs) have stood out amongst EES devices due to their ability to deliver robust power outputs. The performance of the SC technology is dependent on the physicochemical properties of the electrode materials, hence the fine-tuning of such properties will result in enhanced device performance.[2] This work reports on the one-pot hydrothermal synthesis of the nitrogen-doped reduced graphene oxide/hausmannite manganese oxide (N-rGO/Mn_3O_4) nanohybrid as electrode material for supercapacitor application.

The N-rGO/Mn_3O_4 nanohybrid displayed enhanced specific capacitance of 345 F g^{-1}, specific energy of 12.0 Wh kg^{-1} (0.1 A g^{-1}), and a maximum power density of 22.5 kW kg^{-1} (10.0 A g^{-1}) in a symmetric configuration. It also displayed an improved energy density of 34.6 Wh kg^{-1} (0.1 A g^{-1}) in an asymmetric configuration, whilst the maximum power density reached 14.01 kW kg^{-1} at a current density of 10.0 A g^{-1}. The excellent electrochemical performance and capacitive behaviour of the N-rGO/Mn_3O_4 nanohybrid displayed potential for the development of high power and energy output devices.

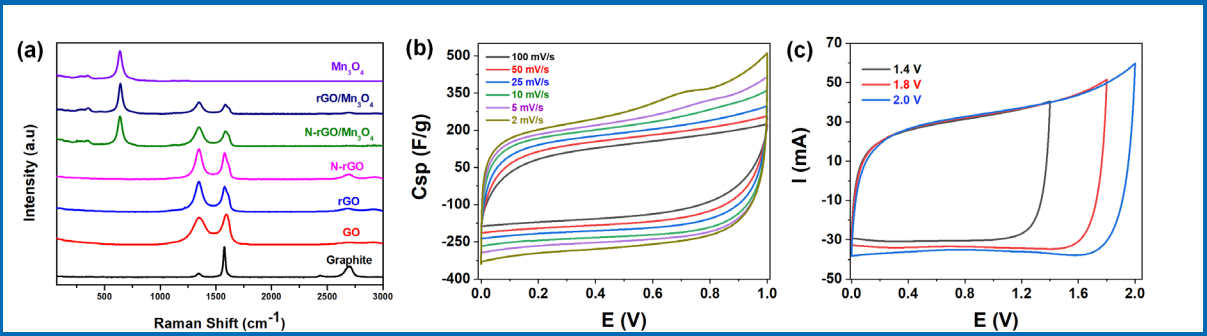


Figure 1: An illustration of (a) Raman spectra of synthesized materials, and cyclic voltammograms of N-rGO/Mn_3O_4 nanohybrid for (b) symmetric and (c) asymmetric configurations.

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INVITED SPEAKERS

Semiconductor Nanowires: A Nanomaterial Platform for Energy Conversion Technologies

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Semiconductor nanowires and nanowires heterostructures provide a formidable playground to explore novel strategies for energy conversion and harvesting. Building on the epitaxial growth of III-V semiconductor nanowires we demonstrate prototypical nanodevices enabling superior control of the thermoelectric figure of merit [1], also resorting unconventional gating approaches which exploit electrolytes [2-4]. Exploiting twining superlattice nanowires, we show ten-fold reduction of thermal conductivity while preserving electric mobility and conductivity as well as Seebeck coefficient [5]. The Soret effect in polyelectrolytes is exploited to engineer heat-driven iontronic transistors based on individual InAs nanowires [6].

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Oxide Perovskites Nanoparticles Thin Films for High LightAbsorption and White Lightsource

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1) Aim and approach

Inorganic thin film PV is mainly based on CdTe, amorphous Si or CIGS. Very recently, hybrid perovskitesemerged with a maximum yield of 23 %.
However, these materials have problems of stability, reliability, toxicity and scale (cell size). Of course, research in this area is focused on solving these challenges, but success is not guaranteed. An alternative route, inorganic oxides, could have significant advantages. The ideal bandgap for an active photovoltaic layer for the solar spectrum is about 1.3 eV. However, oxides with such values are rare. One of the most studied oxides to date as a photovoltaic active layer is cuprous oxide Cu2O. Its bandgap width is around
2.1 eV and is therefore not ideal for the solar spectrum. Conversion efficiencies generally do not exceed 4%. In this project we propose to study a type of emerging solar cell that is based on ferroelectricity. In this type of solar cell, a junction p-n is not necessarily necessary, the opposite conventional solar cells. Interesting conversion efficiencies are starting to be achieved with this type of cell (up to 8.1% in 2015), however the mechanisms are still not well understood and several challenges at the material and engineering levels need to be addressed.
Our aim is to fabricate a novel type of ferroelectric oxides perovskites as thin film form using nanoparticleson silicon and conductive glass (ITO) substrates to improve the light absorption and optical application.

2) Scientific innovation and relevance

Ferroelectrics have recently attracted attention as a candidate class of materials for use in photovoltaic devices, and for the coupling of light absorption with other functional properties [1–3]. In these materials,the strong inversion symmetry breaking that is due to spontaneous electric polarization promotes the desirable separation of photo-excited carriers and allows voltages higher than the bandgap, which may enable efficiencies beyond the maximum possible in a conventional p–n junction solar cell [4–5].Ferroelectric oxides are also stable in a wide range of mechanical, chemical and thermal conditions and can be fabricated using low-cost methods such as sol–gel thin-film deposition and sputtering [3].
The objective of this paper is to initiate an innovative photovoltaic technology based on novel inorganic and multifunctional oxide materials with suitable bandgap widths. These oxides are more stable, need lessperovskites and facile to be integrate in silicon technology. We aim to synthesize ferroelectric materials that absorb a large part of the solar spectrum with reduced bandgap widths and give high Voc value. Our interest was in $Pb(Zn_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PZN-PT) perovskites that revealed excellent ferroelectric,piezoelectric and ferroelastic properties in solid state [7]. However, despite these excellent properties andperspectives to use them in solar cells devices, the veritable challenge is to fabricate them as in thin filmsform because of their incongruent melting point.
To overcome this challenge, oxide perovskites nanoparticles were dispersed in an inorganic gel (for Si substrate) and biopolymer (for ITO substrate). They were deposited by spin coating on nanostructured silicon and ITO substrates. Optical characteristics in UV-Visible and Near IR ranges, photoluminescenceand Raman Luminescence were performed.

3) Results/conclusions/perspectives

The addition of the HTM layer strongly increases the absorption throughout the visible spectrum and IR region as shown in Figure 1. HTM increases the absorption value in the whole visible region (around 100%) and decreases slightly to between 85 and 95 % in IR region. The Mn doping reduces slightly the absorption value in Near IR region while no change is observed in visible one. The results show good perspectives for solar cells application. The biopolymer1 seems to have less influence on the absorption compared with HTM. The same behavior was found for the Silicon nanowires samples with perovskites dispersed on their surfaces. According to the SEM images we obtained thicknesses of 1.600 µm, 1.505 µm and 1.765 µm respectively for ITO, TiO2 and np-PZN-PT-biopolymer1/HTM layers. This allowed us to confirm the value of the thickness of the ITO given by the supplier (1.6 µm). The I-V characterization shows that lightning could improve polarization between 120 to 300 % showing good perspectives for photoferroelectric application. The V_{oc} value is very high (2.1 eV) compared to the silicon one (0.6 eV) for a sample composed to ITO/TiO2/PZN-4.5PT(perovskite)/biopolymer2/HTM/Ag (Figure 2). The I-V curve signs depend to the polarization orientation

Other investigations are in progress especially on the stability in time and temperature.

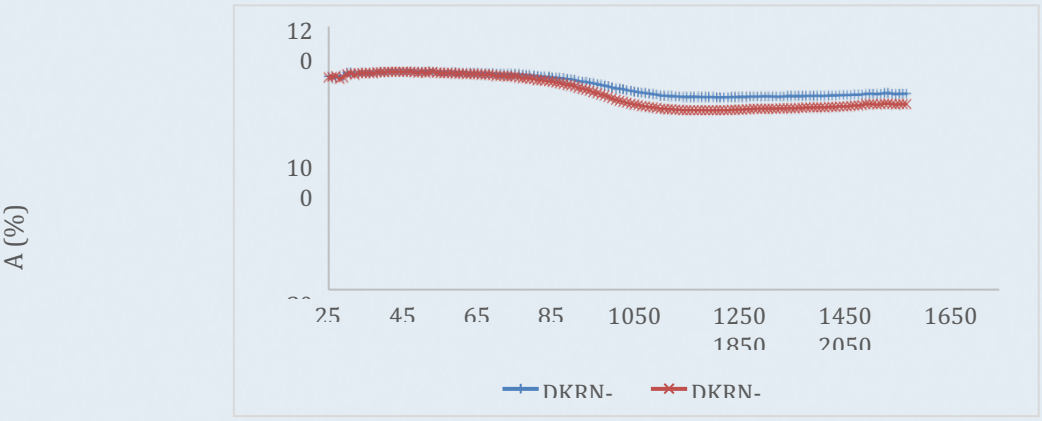


Figure 1: Absorption spectra of undoped (DKRN-ITO7) and Mn doped (DKRN-ITO8) PZN-4.5PTperovskites nanoparticles thin film on ITO substrate.

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Local Plastic Waste Valorization Potential: Fuel Conversion and Characterization

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Plastics generally play a very important role in a plethora of industries, fields and our everyday lives. In spite of their cheapness, availability and important contributions to lives, they however, pose a serious threat to the environment due to their mostly non-biodegradable nature. Recycling into useful products can reduce the amount of plastic waste. Thermal degradation of plastics is becoming an increasingly important recycling method for the conversion of plastic materials into valuable chemicals and oil products. In this work, waste Polyethylene terephthalate water bottles were thermally converted into useful gaseous and liquid products. A simple pyrolysis reactor system has been used for the conversions with the liquid product yield of 65% at a temperature range of 400°C to 550°C. The resultant products have been analyzed via GCMS, FTIR, and GC. A simple pyrolysis reactor system has been used for the conversions with the liquid product yield of 65% at a temperature range of 400°C to 550°C. The chemical analysis of the PET pyrolytic oil showed the presence of functional groups such as alkanes, alkenes, alcohols, ethers, carboxylic acids, esters, and phenyl ring substitution bands. The composition of the pyrolytic oil was analyzed using GC-MS, and it was found that the main constituents were 1-Tetradecene, 1-Pentadecene, Cetene, Hexadecane, 1-Heptadecene, Heptadecane, Octadecane, Nonadecane, Eicosane, Tetratetracontane, etc. The physical properties of the obtained pyrolytic oil were close to those of mixture of petroleum products. The physical properties of the obtained pyrolytic oil were close to those of mixture of petroleum products. The results are promising and can be maximized by additional techniques such as hydrogenation and hydrodeoxygenation to obtain value-added products. This pyrolysis approach provides a promising route to help solve the problem of environmental pollution caused by waste polymeric materials and providing alternative energy needs.

Keywords: Plastic, Pyrolysis, Hydrodeoxygenation, GCMS, FTIR)

Processing Thin and Robust Sulfide and Oxide Solid-State Electrolytes for Lithium Metal Batteries

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Lithium solid-state electrolytes are expected to improve next-generation energy storage technology on the basis of specific energy, safety, and cost. However, there has been limited success in the mass production of solid-state separators with transport properties and comparable thickness to a traditional polypropylene separator used in state-of-the-art lithium-ion batteries. This problem is especially difficult with both sulfide- and oxide-based solid electrolytes, such as lithium argyrodites and lithium garnets, together with integrating effective thin interlayers that enable lithium metal anodes. Several vacuum-based and sol-gel-derived methods have shown promise in making thin solid-state electrolyte films with relatively high ionic conductivity (~10^{-6} - 10^{-5} S/cm at room temperature), yet lithium loss during post annealing can alter the phase as well as significantly affect the lithium transport properties as well as the impedance at the Li||solid-state electrolyte interface. Therefore, the exploration of scalable fabrication techniques is of special importance to develop thin and robust films of sulfide- and oxide-based solid-state electrolytes with high ionic conductivity. In this talk, techniques based on scalable solution-based chemistries will be presented for sulfide- and oxide-based solid-state electrolytes. The crystallization and the phase transformations of the solid-state electrolytes will be discussed based on the concentration of cations and the boiling point of the solvents used in the solution-based chemistries. The results presented in this talk highlight a new opportunity for manufacturing oxide- and sulfide-based solid electrolytes with tunable electrochemical properties, thicknesses, and surface areas. The insights from this work are expected to serve as fundamental guidelines for future optimization toward solution-based processing of superionic solid-state electrolyte materials for next-generation lithium metal batteries.

Acknowledgements
This research was supported by Laboratory Directed Research and Development (LDRD) funding from Argonne National Laboratory, provided by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC02-06CH11357.

Radical Polymer Devices for Energy Storage and Solar Cell Applications

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Organic radical polymers in which each unit is a stable paramagnetic radical that can be reversibly oxidized, reduced, or both, [1] are unique alternatives semiconducting polymers with diamagnetic repeating units that normally exist only with one state, which are at the basis of any polymer organic electronic devices proposed to date, including bulk-heterojunction organic photovoltaics (OPVs) and organic light emitting devices (OLEDs).

While the electrical transport properties in organic semiconductors can be described by the formation of solitons along the polymer chain, or via polarons, the electrical conductivity polyradicals stems the oxidation of a radical site forming a cation, which can oxidize a neighboring neutral site, moving the oxidation even further along the polymer chain in a dynamic redox process described by Marcus electron transfer. This model has enabled the design of organic solar-cell hole transport layers [3] and redox flow batteries a large class of polynitroxide radical polymers [4] with stable neutral (R·) and cationic (R+) states at each repeating unit, such as poly(2,2,6,6-tetramethylpiperidinyloxy methacrylate) (PTMA) poly (4-glycidyloxy-2,2,6,6-tetramethyl piperidine-1-oxyl) (PTEO) and poly(2,2,6,6-tetramethyl-1-piperidinyloxyl) (PTVE). Despite recent claims of p-type polynitroxyl doping [2], all such materials have so far fallen short of enabling any electronic devices, such as organic field effect transistors (OFETs) in which gate modulation and differentiated p-type and n-type transport electrons and holes is necessary.

In this talk, we will review our work [3,4] on electrotunable radical polymers with ambipolar characteristics, in particular poly-(oxo)verdazyls in which each repeating unit may stably exist in the anionic (R-), neutral (R·) and cationic (R+) configuration. We show that due to the possibility of reversible disproportionation and comproportionation (2R· « R+ + R-) along the polymer chain enables both ambipolar and p-type field effect transistors. Furthermore, the same systems can be utilized in single-layer flow batteries, resistive memory devices and hybrid solar cells. The competitive advantages of tri-stable poly-(oxo)verdazyl radical polymers, stemming from their behaviour as strongly correlated systems will be discussed along their foreseen applications.

Keywords: Radical polymers, Materials for electronics, Energy storage, Solar cells

Acknowledgement: The hard work of graduate students and postdocs from my group (specifically: S Ezugwu, D Singh, P Bazylewski, E Aawani, S Catingan, M McCready, J Park and V Wong) is gratefully acknowledged. Gilroy's group from Western's Chemistry Department (in particular: J Paquette, F Magnan, M Anghel and J B Gilroy) is gratefully acknowledged for their synthetic chemistry contributions to this project.

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Nanocrystalline Materials for Photovoltaic Applications: Perovskites and Chalcogenides

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Nanostructured materials possess interesting properties researchers seek to overcome current technological challenges. Improving the performance of existing or new devices is the main aim set by scientist when studying nanoparticles. Inorganic perovskites and copper indium selenide nanocrystals were prepared via classical colloidal method and microwave assisted method.Various parameters of synthesis including the time, temperature, precursor concentration, coordinating solvent and capping agent were investigated. Their properties were studied and optimized for effective application in photovoltaic devices. Several types of solar cell devices as well as perovskite cells were prepared from thin film of synthesized nanocrystals and the evidenceof photovoltaic activity was shown. The performance of fabricated devices was influenced by thestructure of deposited thin films, especially the absorbing layer made of synthesized nanocrystals.

Keywords: nanocrystals, synthesis, energy

Progress in Batteries for Electric Cars

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There have been many reports of fire caused by the batteries in electric cars! This has led to a search for other types of cathodes that do not contain any oxygen. The inductive effect from (PO4)3-ions increases redox potential (compared to those in oxides) and stabilizes the olivine structure. LiFePO4 (LFP), is fire-resistant and non-combustible. We first reported our synthesis of LFP in 2012 (Characterization of LiFePO4/C cathode for lithium ion batteries; Lyczko N,Nzihou A,Sharrock P,Germeau A,Toussaint C, Ind.Eng chem Res,51,2012). The main problem with LiFePO4is its low electronic conductivity. Both ionic and electronic transport need to be improved simultaneously and can be obtained by reducing the size of primary particles. It had also been reported that carbon coating on LiFePO4particles was effective in improving its electrochemical performance so we added carbon black and ball-milled it. XRD patterns of LiFePO4/C were obtained for samples heated up to 650°C. An olivine crystal structure shwed good agreement with the literature with cell parameters: a = 0.60 nm; b = 1.03 nm; and c = 0.47 nm. This product corresponds to well crystallized LiFePO4in a single phase. The EDX analysis of LiFePO4/C showed the expected atomic percentages. This confirmed the stoichiometry of LiFePO4.An experimental battery was made with 80% of the prepared LiFePO4mixed with 10% carbon black and 10% polyvinylidene fluoride as binder. The galvanostatic charge-discharge tests were performed and best results were obtained with powders calcined to 650°C with 147 mAh/g. We feel that decreasing the particle sizes and control of porosity should better results by facilitating ion diffusion. We compare LiFP results and show they are safer, less expensive and as good as standard LiCoO2.

Keywords: Lithium-Ion Batteries. LFP: Cathodes with No Oxygen

Metal Oxide Ion-Gated Transistors: Interfaces, Electronic Properties and Applications in Printable Electronics and Energy Storage

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Ion-gated transistors (IGTs) operate through the interface between a transistor semiconducting channel material and a gating medium containing mobile ions. IGTs have been investigated for printable and flexible electronics as well as synaptic devices.
The structure and the dynamics of electrical double layers at ionic gating media-semiconducting transistor channel interfaces govern the working mechanism of IGTs.
Atomic Force Microscopy Force-Distanceprofiling on those electrical double layers permits to follow, in operando conditions, the evolutionof the arrangement of the ions at the interface with the channel material.
Capitalizing on such fundamental scanning probe studies and following the time response of the transistor characteristics under electrical bias, we propose to extend the application of IGTs to electrochemical energy storage.
Here, IGTs could be used as in situ diagnosis tools to follow the state of health of battery metal oxide cathode materials with the aim to prolong the life time of the battery and plan any possiblesecond use of the battery itself or its constituting materials.

Keywords: Transistors, Ion Gating Media, Electrical Double Layers, Metal Oxides, Li-Ion Batteries

Performance Evaluation of Bi_2O_3@GO and Bi_2O_3@rGO Composites Electrode for Supercapacitor Application

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Among other energy storage systems, supercapacitors have been of higher research interest for optimal energy utilization due to their outstanding intrinsic properties such as; high electrical response, great durability, a wide range of operating temperature and voltage. In this work, synthesis and comparison of the electrochemical performances of graphene oxide doped with Bismuth oxide (Bi_2O_3@GO) and reduced graphene oxide doped with Bismuth oxide (Bi_2O_3@rGO) without any binder material were carried out using a very low concentration (1.0 M) of KOH electrolyte, the solvothermal method of nanomaterial synthesis was employed. The produced materials were studied using X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FT-IR), and electrochemical characterizations. An improved performance was recorded by the electrode made of Bi_2O_3@rGO which achieved; 560 Fg^{-1} specific capacitance at 5 mVs^{-1} scan rate, 280 $Whkg^{-1}$ and 40 $kWkg^{-1}$ energy and power densities respectively, the electrode also retained 99% of its capacitance after 3000 galvanostatic charge-discharge (GCD) cycles.

Keywords: Bismuth oxide; Graphene oxide; Composite; Electrochemistry; Supercapacitor



ORAL
PRESENTATERS

Interface Engineering of Cesium–Containing Triple Cation Perovskite for Highly Efficient and Stable Inverted Solar Cells

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The paper presents the effects of sodium heptadecafluorobutyrate molecule as a passivation layer to achieve enhanced stability in cesium-containing triple cation perovskite solar cells. The molecule, easily dissolved in a polar solvent readily wetted the surface of the perovskite absorber layer providing improved surface coating. The molecular conformed devices maintained exceptional stability over the 180 s for the maximum power point tracking with a power conversion efficiency of ~22.51%. Longevity in the efficiency of perovskite solar cells are due to the strong passivation by the fluoride ion, interfacial contacts and dipole interactions. The results are discussed to elaborate on the bond strengthening of fluoride ions and the enhanced stability and high efficiency of inverted triple cation perovskite solar cells.

Keywords: *Passivation, Dipole Moments, Interface Engineering, Perovskite Solar Cells.*

Sustainable Development of Ni-VO_2@Carbon Composites Derived from Cashew Leaves for Application in Supercapacitors

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Herein, we successfully fabricated a hierarchically structured three-dimensional, Vanadium dioxide composites (VO_2@C and Ni-VO_2@C) via a one-step green solvothermal process from cashew leaf. X-ray diffraction (XRD), Raman spectroscopy, scanning electron microscope (SEM), gas adsorption/desorption analysis and X-ray photoelectron spectroscopy (XPS) were used to confirm the incorporation of carbon in the VO_2 matrix as well as the successful doping with Nickel. The electrochemical performance of the composites was evaluated in a three-electrode configuration using 6 M KOH aqueous electrolyte. The Ni-VO_2@C composite exhibited a very good capacitance of 355.2 $F.g^{-1}$ (49.3 $mAh.g^{-1}$) with an excellent columbic efficient of 97.3% at 10 $A.g^{-1}$. To evaluate practical application, an asymmetric device was fabricated using Ni-VO_2@C composite as the positive electrode and activated carbon (AC) as the negative electrode. The assembled device exhibited an energy density of 21 $W.h.kg^{-1}$ and an excellent power density of 972 $W.kg^{-1}$ at a cell voltage of 1.6 V at a specific current of 1 $A.g^{-1}$. Moreover, long term device stability was exhibited with an 88% capacitance retention over 10 000 charge/discharge cycles at 10 $A.g^{-1}$. The remarkable electrochemical performance based on the good synergy between VO_2 and carbon, and the effect of Nickel doping, indicating that this Ni-VO_2@C composite could be used to develop advanced cathode for next generation of supercapacitors applications.

Keywords: Supercapacitor, biomass, carbon, VO_2(B), Nickel

Resilient Masonry for Low Income Housing: An Exploration of the Cold Sintering Process Using Wollastonite ($CaSiO_3$)

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Aligning the built environment with the United Nations Sustainable Development Goals and the Sendai Framework for Disaster Risk Reduction requires resource efficient material production strategies. Bricks and ceramics are integral part of building envelopes around the world. They are produced through energy inefficient processes. For example, commonly used bricks are usually fired at between 900 and 1000 degrees Celsius. As part of previous research efforts, we have sought to address this problem through investigating the use of unfired compressed earth bricks. One of the challenges associated with the production of compressed earth bricks is the scale of production. In this current research, we are exploring the feasibility and viability of using the Cold Sintering Process to produce high quality bricks at room temperature. The input material is Calcium Silicate ($CaSiO_3$). Our findings demonstrate that the CSP could yield sustainable and resilient masonry units.

Keywords: resilient materials, sustainability, climate action, low carbon materials.

Solar Cells and Thin Films Made from Halide Perovskites Show Abnormally High Resistance to Alpha Irradiation in Radiation Areas

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Solar cells (SCs) and thin films made of methylammonium lead tri-iodide ($MAPbI_3$) demonstrate remarkable robustness when irradiated with alpha radiation (He^{2+}) from americium-241 (^{241}Am). A study of the structure, absorption, and surface morphology of perovskite thin films, and the photoelectronic properties of SCs have been conducted with and without irradiation with He^{2+}. According to XRD analysis, tetragonal $MAPbI_3$ showed increased crystallinity and a decrease in compression micro-strain, with an increased flux of He^{2+}. There was no significant difference in UV-Vis absorption until the flux exceeded 7.36 x 10^{12} He^{2+} cm^{-2}. Bandgaps for irradiated films decreased similar to those for non-irradiated films up to a dose of 3.07 x 10^{12} $He^{2+}cm^{-2}$, but after that, there were large differences. Digital camera photographs showed changes on the thin films irradiated at fluences exceeding 3.07 x 10^{12} He^{2+} cm^{-2}, and micrographs from scanning electron microscopy confirm the changes were caused by pits forming in grains. $MAPbI_3$ SCs maintained 92.3% of their initial PCE under an accumulated dose of 3.07 x 10^{12} He^{2+} cm^{-2} in ambient conditions. We found that $MAPbI_3$ thin films and SCs can survive doses of He^{2+} of up to 3.07 x 10^{12} He^{2+} cm^{-2} in space and He^{2+} radiation environs.

Keywords: Robust $MAPbI_3$ thin film, Alpha irradiation, Robust $MAPbI_3$ solar cell, Space environs, Radiation environs.

Combustion Performance of Solid Refuse Fuel-Derived Biochars for Energy Production

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A drastic reduction in greenhouse gas emissions in the short term is required. In this context, high carbon industrial processes, typically using fossil fuels, should move towards the use of alternative renewable fuels. Biochar obtained from biomass through thermochemical processes, such as pyrolysis can play a role, as it has thermal and processing properties closer to those of coal, which makes it a suitable biosourced alternative to fossil fuels at industrial scale [1]. This work aims at studying biochar combustion, to be used for energy application in various industries. To do this, biochar from Solid Refuse Fuel (SRF) was produced by carbonization, followed by a devolatilization step (650 to 850°C). Biochar samples were characterized in terms of structural properties (BET, microscopy), chemical composition (CHNS, ICP-OES, FTIR), and thermal behavior (TGA-DTG, calorimetric bomb). The results obtained showed that an increase in the devolatilization temperature resulted in a higher C/H ratio. Under an inert atmosphere, the thermal behavior of carbonized SRF was shown to be similar to that of hard coal. TGA-DTG combustion experiments were carried out at different heating rates (5, 10, and 20 °C.min^{-1}), revealing fixed carbon oxidation. Combustion performance was evaluated through the combustion performance index (S), the maximum reactivity (Rmax), and the ignition index (D) [2]. Thus, the ignition temperature rose from 267 °C to 320 °C for carbonized SRF after devolatilization at 750 °C. The fate and quality of emissions versus the composition of the initial feedstocks will be discussed.

Keywords: combustion, carbonization, devolatilization, Solid Refuse Fuel (SRF), emissions

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Synthesis and Characterization of Caesium Lead Tri-Iodide by Sequential Physical Vapour Deposition for Solar Cells

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The sequential physical vapour deposition technique was used to grow quality thick films of metal halide perovskites in a safe, scalable, and reproducible manner. The growth of high-quality poly-crystalline yellow phase caesium lead tri-iodide ($CsPbI_3$) was refined by varying the CsI thickness from 200 nm to 500 nm. Crystallographic parameters and phase transitions from as-deposited orthorhombic γ-$CsPbI_3$ to tetragonal β-$CsPbI_3$ on annealing at 100 °C, were determined using X-ray diffraction patterns. Computed lattice constants were a= 4.88 Å, b= 9.96 Å, and c= 16.52 Å,with an average crystallite size increasing from 169.46 nm to 243 nm, and the micro-strains decreased with an increase of CsI thickness. The field-emission scanning electron micrographs showed a uniform surface covered with polycrystalline grains. The average grain size increased from 168 to 235 nm as the caesium iodide (CsI) thickness increased, resulting in large pin-hole- free and tightly packed grains. A 2.24 to 2.38 eV increase in the bandgap was observed when CsIthickness was increased. Herein, we demonstrated optimized structural, morphological, and optical properties of $CsPbI_3$ for use in solar cells, grown via sequential physical vapour depositiontechnique for stable and completely inorganic perovskites.

Keywords: Cesium Iodide, Sequential physical vapour deposition

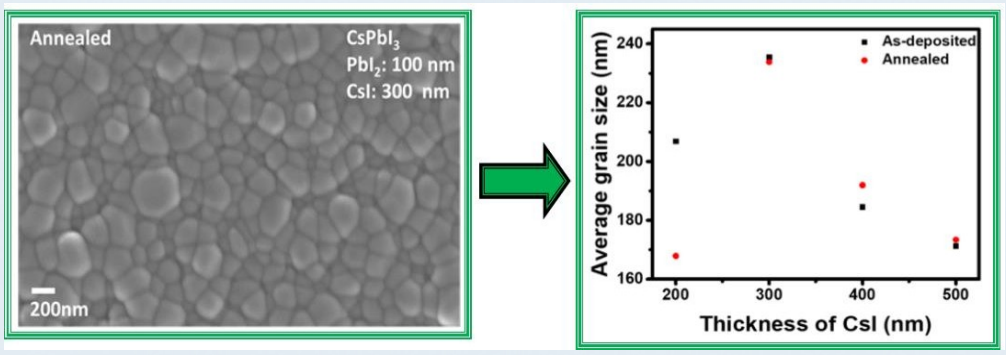


Figure 1: Distribution of $CsPbI_3$ average grain-size (nm) with varying CsI thickness (from200nm - 500nm) in steps of 100.

Biomass Valorisation of Marula Nutshell Waste into Nitrogen Doped Activated Carbon for High Performance Supercapacitors

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This study reports on the valorisation of marula nutshell waste into a valuable electrode material for supercapacitors. Marula nutshell waste, a brown hard residue from marula fruits has been valorised into a nitrogen-doped activated carbon (N-ACs) by KOH treatment and using melamine as a nitrogen source. The microporous and mesoporous nature of N-ACs exhibited a high surface area of 1427 m^2/g and pore volume of 0.31 cm^3/g. the material was analysed in a two-electrode system using 2.5 M KNO_3 electrolyte. The high surface area, the efficient presence of micropores and mesopores, defects, and the high content of nitrogen (5.1%) revealed that the material produced an outstanding energy density of 28.4 Wh/kg and a power density of 499 W/kg in 2.5 M KNO_3 electrolyte. The conversion of marula nuts waste into N-ACs is thus seen to provide a means of converting biomass waste into a useful energy storage material for supercapacitors.

Keywords: Marula nutshells; KOH activation; nitrogen doping; supercapacitors

Photosynthesis Re-Wired on the Pico-Second Timescale

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Photosystems II and I (PSII and PSI) are the reaction center-containing complexes that drive the light reactions of photosynthesis and underpin life on Earth. PSII performs light-driven water oxidation (quantum efficiencies and catalysis rates of up to 80% and 1000 $e^- s^{-1}$, respectively) and PSI further photo-energizes the harvested electrons (quantum efficiencies of ~100%). The impressive performance of the light-dependent components of photosynthesis has motivated extensive biological, artificial and biohybrid approaches to 're-wire' photosynthesis to enable higher efficiencies and new reaction pathways, such as H_2 evolution or alternative CO_2 fixation. To date these approaches have focused on charge extraction at the terminal electron quinones of PSII and terminal iron-sulfur clusters of PSI. Ideally electron extraction would be possible immediately from the photoexcited reaction centers to enable the greatest thermodynamic gains. However, this was believed to be impossible because the reaction centers are buried around 4 nm within PSII and 5 nm within PSI from the cytoplasmic face. Here, we demonstrate using *in vivo* ultrafast transient absorption (TA) spectroscopy that it is possible to extract electrons directly from photoexcited PSI and PSII, using both live cyanobacterial cells and isolated photosystems. We postulate that some quinones can oxidize peripheral chlorophyll pigments participating in highly delocalized charge transfer (CT) states after initial photoexcitation. Our results open new avenues to study and re-wire photosynthesis for bioenergy and semi-artificial photosynthesis.

Keywords: Spectroscopy, Biological physics, Electrochemistry

A Review on Inorganic Tin Halide ($ASnX_3$) Perovskite Solar Cell: Efficiency and Stability

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Tin halide perovskites are a less toxic alternative to lead halide perovskites. This class of metal halide perovskite maintains almost all the desirable optoelectronic properties of lead halide perovskites and boast of the highest efficiency (~14.81 %) out of all lead-free metal halides perovskites. However, its stability in ambient environment is a great challenge, the desirable electrical properties of the solar cells are altered due to Sn^{2+} oxidizing to Sn^{4+} thus limiting the power conversion efficiency and its long-term operational stability. Recent reports show that the choice of A site and X site greatly influence the material stability and performance. Organic cations (CH_3NH_3 , NH_2CHNH_2) occupying A sites are susceptible to degradation because of their high hygroscopicity however inorganic cations (Cs, Rb, K, Na) at A sites have been shown to exhibit better thermal stability. Several research are currently geared towards building up on this advantage of inorganic tin halide perovskites material via additive engineering, partial cation and anion exchange, device architectures, transport layers and processing routes. In this work we summarize the research efforts both experimentally and computationally to enhance the stability and efficiency of all inorganic Sn halide perovskite's materials and solar cells via additive engineering, partial substitution of A and X sites ions and charge transport layers. A brief perspective on the most promising route for enhancing the stability is discussed.

Keywords: Stability, inorganic, tin halide, perovskites solar cells and additives.

Thermoelectric Composites with Magnetically-Ordered Inclusions: State of the Art and Perspectives

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Recently, a new approach toward improving the figure of merit ZT of thermoelectric materials, which consists of introduction of nanosized magnetically ordered inclusions into the bulk matrix of a thermoelectric material, has been arisen. Such a strategy makes it possible to effectively influence the electronic and phonon transport of the composites due to the effects of enhanced phonon scattering, localization and filtering of charge carriers, as well as the paramagnon drag. Application of these approaches has yielded outstanding results for skutterudites [1], NiTiSn-based Heusler alloys [2], tin selenide [3], manganese silicide [4] and tellurides [5,6]. Given the novelty of this approach and its enormous practical potential, research in this direction has attracted growing attention.
In our talk we shall overview achievements in this field and underline the roles played by magnetism in optimization of thermoelectric properties. Besides, original results on the properties of composites based on low- (bismuth tellurides) and medium-temperature (Heusler alloys) thermoelectric matrixes with nanoscale inclusions of magnetically ordered metals and alloys shall be presented and the perspectives of this approach for improving ZT shall be discussed.

Acknowledgment:
This work was supported by the Priority-2030 program of Belgorod State University (project No. 122030200152-0).

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Mixed-Phase Bismuth Ferrite- Carbon Black Nanocomposites by Green Approach as an Efficient Electrode Material for Supercapacitor Application

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Electrochemical supercapacitors have fascinated abundant consideration because of their capacity to distribute high power and energy densities with owing cycling strength[1-2]. The fast growth of research in the field of electrochemical energy storage systems has been determined by the increased development of nanostructured materials[3]. The use of nanomaterials in energy storage and conversion represents anopportunity to advance the performance, density and ease of transportation in renewable resources[4]. In focus of this work is to synthesize the bismuth ferrite- carbon black nanocomposites by green approach via Moringa Olefeira natural extract as an electrode material for supercapacitor application. Supercapacitor performance of a nanomaterial either in the form of a thin-film or a pallet, used as an electrode can be evaluated by cyclic voltammetry (CV) and galvanostatic charge-discharge measurements. The electrodes are prepared by coating the resulted slurry (bismuth ferrite- carbon black) on the surface area of the glassy/platinum electrode by the drop casting process. Their electrochemical activity, crystalline structure, morphology, isothermal behavior and opticalproperties will be studied using various characterization techniques such as X-ray diffraction (XRD) and Energy Dispersive X-ray Spectroscopy (EDS) cyclic voltammetry (CV), galvanostatic charge-discharge (GCD) and electrochemical impedance spectroscopy (EIS) Fourier transform-infrared (FTIR), High Resolution Transmission Electron Microscopy (HRTEM, Differential scanning calorimetry/thermogravimetric analysis (DSC/TGA) Ultra-violet visible (UV-vis) and Photoluminescence(PL).

Keywords: charge-discharge, bismuth ferrite, Green chemistry, Moringa Oleifera, carbon black, supercapacitors

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The Crucial Role of the Binder in Biochar Briquetting for Sustainable Energy Production

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Fossil-based CO_2 emissions need urgently to be reduced to fight against global warming and the associated degradation of the environment. Biochar produced by biomass pyrolysis is a promising sustainable fuel alternative with a high fixed carbon and a relatively low volatile matter and ash content. However, densification is required to overcome its low density, which is the main inconvenient for its use. In this sense, briquetting forms biochar agglomerates with a suitable size, shape, density, composition and energetic content, which eliminates challenges associated with transportation, storage and handling of powdered material. In addition, it improves the fuel's energy density, hydrophobicity, mechanical strength and durability.

The choice of the binder in biochar agglomeration is critical for guaranteeing optimal mechanical properties with fewer emissions and without compromising the calorific value. According to the literature, the most interesting binders for biochar densification include organic compounds, such as starch, molasses, lignin, and bio tar, and inorganic compounds, such as cement, clay, lime, plastic waste, and asphalt. Co-densification combining organic and inorganic binders would benefit from their synergic interaction leading to improved combustion and mechanical properties [1]. The operating conditions of the combustion process of the densified biosourced fuel need to be well controlled in terms of Quality, Health, Safety & Environment (QHSE). Common emissions are SO_2, NO_x, particulate matter, and volatile organic compounds (VOC). Their severity depends on the biomass type and the chemical composition of the briquette, including the binder [2].

In this context, the aim of this study is to prepare and optimize the formulation of biochar briquettes from renewable raw materials and binders, so as to propose an alternative biosourced fuel. Preliminary results showed that biotar, starch and lime produce briquettes with high strength and high calorific value when properly formulated in the biochar composite.

Keywords: Biochar, briquetting, binder, biotar

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Decoupling Proton and Cation Contributions to Capacitive Charge Storage in Birnessite in Aqueous Electrolytes

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Nanostructured birnessite (δ-MnO_2) is of interest as an electrode for aqueous electrochemical energy storage due to its high specific capacity and nearly ideal electrochemical capacitive behavior. The mechanism of electrochemical capacitance in birnessite has been described as both Faradaic (involving redox) and non-Faradaic (involving only electrostatic interactions). Both protons and cations contribute to the charge storage mechanism of birnessite in neutral pH aqueous electrolyte, whereby structural changes from intercalated cations are mitigated by interlayer structural water. To fully understand the charge storage mechanism, the role of protons in aqueous electrolytes must be further examined. The hypothesis guiding this study is that protons are contributing to the specific capacity of birnessite through proton-coupled electron transfer (PCET) reactions occurring at the surface. To investigate these PCET processes, we explore the electrochemical response in neutral pH electrolytes at varying buffer concentrations. The addition of buffer to the electrolytes increases the amount of available protons in solution without a pH change, allowing for additional proton transfer, and therefore additional charge storage. By utilizing our understanding of PCET reactions in buffered electrolytes, we can decouple the role of protons and cations in the capacitive charge storage mechanism of birnessite. Our findings show an initial increase in capacity upon the addition of buffer, with higher buffer concentrations resulting in higher capacity. Cyclic voltammetry shows a slight increase in specific current as buffer concentration increases, as well as the onset of new redox peaks, indicative of the presence of PCET reactions occurring on the surface or within the interlayer of birnessite. Long-term cycling in buffered electrolytes leads to rapid film dissolution and capacity decay, which is supported by ReaxFF atomic scale simulations. This presentation will provide an understanding of the proton and cation contributions to the charge storage mechanism of birnessite in neutral pH electrolytes.

Keywords: Birnessite, Capacitance, Cyclic voltammetry, Desalination, Energy storage

Cycling Demonstration of Sequential Deposition Synthesized Lithium Garnet Films in Full Batteries

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Sequential deposition synthesis (SDS) is a recently-discovered technique that allows a solid-state electrolyte layer to be fabricated directly from a liquid precursor which is then atomized onto a heated substrate where the solvent evaporates and the precursor salts decompose to form a conformal layer. $Li_7La_3Zr_2O_{12}$ (LLZO) is a promising material that has seen much interest in the battery field but has challenges to synthesize this layer between 5-15 µm thick which SDS is capable of fabricating. LLZO films were fabricated directly onto a porous substrate that was infiltrated with a polymer gel electrolyte and the cycling performance was demonstrated in a full cell using Li metal anode and lithium cobalt oxide (LCO) cathode. The cycling performance is discussed in reference to state-of-the-art performance in the battery field and post-mortem analysis on the cells is performed to elucidate failure mechanisms.

Keywords: Solid-state electrolyte, spray pyrolysis

Understanding Gas Evolution and SEI Formation in Hard Carbon Anodes in Sodium Ion Batteries Using Sensitive Instantaneous Electrochemistry Mass Spectrometry

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In the exploration of alternative battery technologies to allow for diversification from lithium-ion batteries, there is the need to fully understand current contending technologies to develop, improve their performance and eventually scale up. Consequently, in-operando studies are the ideal method to better understand battery behavior, however setting up these techniques can be complex and not entirely representative. (1) Sodium ion batteries are considered a competitively applicable technology for varied utilization due to their similar chemical properties to lithium. These similarities also make it easy to transfer technologies on a larger industrial scale. Sodium ion batteries however differ from lithium in their degradation mechanism due to an increased reactivity of sodium. As a result, the solid electrolyte interface is less stable and more reactive, while the carbonate electrolyte commonly used in both systems have been shown to decompose more favorably in sodium batteries. In addition to this, side reactions aiding degradation are observed in sodium batteries. (2) Here, we introduce a novel electrochemistry mass spectrometry technique in the study of degradation mechanisms and gas evolution in sodium ion batteries, initially focusing on the hard carbon anode. (3)This technique analyses the gases evolved during electrochemical cycling in a time sensitive manner, using a specially designed cell attached to the mass spectrometer, in addition to a micro-fabricated silicon membrane chip which allows for instantaneous transfer of volatile species from the cell to the mass spectrometer without differential pumping, thereby reducing loss of analyte and allowing for faster detection and more accurate analysis. Combined with other surface and electrochemical characterization techniques, this technique gives insight to the degradation mechanisms and SEI formation mechanisms in sodium ion batteries.

Keywords: Mass Spectrometry, Electrochemistry, Sodium Ion Batteries, Hard Carbon

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Boosting Oxygen Reduction Catalysts with Optimal Mesoporosity of Carbon Support

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The extensive application of proton exchange membrane fuel cells (PEMFC) is conditioned by the limited supply and high cost of the Pt used in commercial PEMFC catalysts. To make PEMFC more widely available, new electrocatalysts with low Pt loading and high Pt efficiencies must be developed.

An important, but little explored aspect of this, is the interaction between the carbon support, proton conductive ionomer and catalyst. Catalyst support with optimal porosity is suggested to protect the Pt particles from direct ionomer poisoning but still provide the particles with good accessibility to the protons and oxygen.

In our project, carbon nanospheres with highly ordered mesoporous channels have been synthesised sustainably from biomass. Pt nanoparticles were deposited via polyol method onto the as synthesised mesoporous carbon sphere (MCS) and another two commercially widely used carbon substrates (porous Ketjenblack and non-porous Vulcan). Characterization of the catalysts were carried out with SEM/TEM, BET, XPS, XRD, revealing that the Pt nanoparticles are same in geometric and electronic structure while the difference of these catalysts solely arises from the different support porosity thus the different local environment of Pt NPs in the catalysts. All the Pt/C catalysts were tested under a gas diffusion half-cell configuration for their oxygen reduction performance. Pt/MCS shows supreme performance where the Pt NPs sit inside the mesoporous channels of the carbon sphere.

To understand the outstanding activity of Pt/MCS, *operando* X-ray Absorption Spectroscopy was used to evaluate the ionomer coverage on the Pt surface by monitoring the Pt electronic structure change in the potential range of 0.1-1 V (vs RHE). We proved that the oxygen reduction performance was boosted via the ideal interaction of Pt and Nafion ionomer, where direct contact in-between these two is eliminated without sacrificing the accessibility of Pt active sites. This will then guild the design strategy for future electrocatalysts development.

Porous Carbon Derived from Washingtonia Robusta Barks for Supercapacitor Device Applications

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This study presents porous carbon derived from Washingtonia Robusta barks (Mexican fan palm) by hydrothermal pretreatment reaction followed by KOH chemical activation and its application in supercapacitor device. Various activation parameters, including KOH to carbon (KOH/C) impregnation ratio, time and temperature on the device's electrochemical performance, were investigated. The electrochemical studies revealed that the specific capacitance was affected by activation temperature, impregnation ratio and time. Increasing both activation temperature and time favored performance of the device prepared with samples with impregnation ratio 1. However, specific capacitance decreased with increasing activation time for samples synthesized at KOH/C ratio of 2 and 3 at all activation temperature. The fabricated device with HHPB sample prepared with KOH ratio 3 at 700°C for 60 minutes attain specific capacitance of 179.3 and 169 F/g at scan rate of 5 mV/s and current density of 0.5 A/g respectively, good cycling stability with 95% capacitance retention and 100% coulombic efficiency when cycled 5000 times at current density of 2 A/g. HHPB electrodes reveals perfect EDLC behavior with energy density of 20 Wh/kg and power density of 2000 W/kg when used in symmetric coin supercapacitor cell with 6 M KOH solution. These findings show the potential of fan palm barks as electrode materials with good stability and high-rate capability for supercapacitor application.

Keywords: Porous carbon, palm bark, Washingtonia, capacitance

Flexible Organic-Inorganic Photovoltaic Characterization

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Commercial production of electronic devices on deformable and flexible substrates has become a critical requirement for large-area electronics, such as electronic textiles, electronic papers, sensor skin for robotics, and wrap-able solar cells or flexible displays. In this research, a three-point bending process is used to investigate the optical, electrical, structural, and mechanical properties of organic-inorganic-based flexible electronics. The relationship between the optoelectronic performance of the various device layers will be studied. The effects of stress and strain on the current-voltage characteristics of the device modeled using the density functional theory technique show how the optoelectronic properties are affected before and after the bending processes. The device structure, flexural strength, and their applications in the commercial production of flexible electronics are discussed.

Keywords: Flexible, optoelectronics, electronic device.

Biomass To Energy an Opportunity in Casamance Region (Senegal)

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Providing a solution to deforestation is an environmental issue for the development of the developing countries, especially those in the south. Yet, a significant part of the forest has disappeared quite rapidly in recent years. Environment problems are compounded by health problems. According to 2012 WHO reports, 1.6 millions of women and children die each year from wood and charcoal smoke. So, we are all concerned because one of the most worrying threats at the moment is global warming due to greenhouse gas emissions. Open burning of agricultural residues and deforestation for the production of firewood and charcoal make the recycling and conversion of biomass waste a priority. Moreover, Biomass valorization can be a solution to generate revenue from agro-forestry waste and to produce Green Energy in order to protect the global environment because the awareness of *using* Eco-friendly & Non-conventional Bio-coal / Bio-fuel is increasing day-to-day due to the increasing of the conventional fuel cost.

Africa is a region with the most significant amount of underutilized renewable energy sources, but … slow at mobilizing this potential.

However, the establishment of sustainable technologies adapted to the recovery of such residues requires prerequisites of technical (conversion costs related to conversion technologies, biomass costs and fossil fuels price) and regulatory (Public policies that affect supply and demand and in some cases the cost of biomass and climate regulations).

And it is in this sense that we try to make our contribution so that this renewable energy obtained from biomass move to bioenergy and biochemicals nationally, regionally and globally.

High electrochemical performance of the Nickel cobaltite@biomass carbon composite (NiCoO@BC) derived from bark of Anacardium Occidentale for supercapacitor application.

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In order to achieve a high energy density without degrading the great power density of supercapacitor, one of the best strategies is to compound carbon-based materials with pseudocapacitive materials. Biomass carbon-based materials are promising for supercapacitors applications owing to their high carbon yield and low-cost. In this work, an easy energy-saving hydrothermal process was used to synthesize nickel cobaltite with biomass-derived carbon (NiCoO@BC). The structural and morphological properties were characterized by XRD, Raman spectroscopy, SEM, TEM and XPS techniques. The electrochemical performances investigated in a three-electrode configuration using 6 M KOH aqueous electrolyte and a working potential of 0.5 V (vs Ag/AgCl) reveal a pseudocapacitive behavior. The composite displays a specific capacitance of 475 F g^{-1} at a current density of 0.5 A g^{-1} and good cycling stability with a coulombic efficiency of 98% and capacitance retention of 72% after 7000 charge-discharge cycles at a current density of 10 A g^{-1}. For practical application an asymmetric device was assembled using NiCoO@BC composite as positive and activated carbon as negative electrodes. The device delivered a good energy density of 20 W h kg^{-1} at a power density of 897.9 W kg^{-1}. The excellent cycling stability with a coulombic efficiency of 99% and a capacitance retention of 78% up to 15000 cycles indicates that the composite Nickel cobaltite@biomass carbon is a promising candidate as electrode materials for next supercapacitors generation.

Keywords: Supercapacitors, Electrochemical performances, Nickel cobaltite@ biomass carbon

Low Temperature Thermally Reduced Graphene Oxide Directly on Ni – Foam Using Atmospheric Pressure – Chemical Vapor Deposition for High Performance Supercapacitor Application

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In this paper, thermally reduced graphene oxide (TRGO) at 200 ℃ directly on Ni – Foam (NF) (current collector) was prepared via atmospheric pressure – chemical vapour deposition (AP – CVD) and used as a positive electrode for supercapacitor application. The TRGO/NF electrode preparation method is simpler, quicker, cheaper and more effective compared to the traditional slurry pasting method. The half-cell electrochemical performances in 6 M KOH showed a maximum specific capacity of 52.64 mA h g^{-1} at 0.5 A g^{-1}. The device: TRGO/NF// PAC showed a specific energy and power of 18.72 W h kg^{-1} and 547.52 W kg^{-1} respectively at 1 A g^{-1}; and 14.10 W h kg^{-1} and 2.5 kW kg^{-1}, respectively at 5 Ag^{-1}. The high coulombic efficiency (99.9%) and capacitance retention (80%) indicate outstanding stability. These results represent a significant progress in the fabrication of binder and conductive enhancement free positive electrode for electrochemical energy storage devices.

Keywords: Thermally reduced; Energy storage; Chemical Vapor Deposition; Ni – Foam; Binder – free supercapacitor

Vanadium Dioxide Sulphur-Doped Reduced Graphene Oxide Composite as Novel Electrode Material for Electrochemical Capacitor.

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Vanadium dioxide presents considerable electrochemical properties such as non-toxic, multiple oxidation states and good specific capacity/capacitance, thus a good candidate for supercapacitor applications. However, it is obstructed by low electrical conductivity and lack of cycling stability as compared to carbon-based materials. Reduced graphene oxide (rGO) possesses excellent supercapacitor properties, such as high specific surface area, good electrical conductivity and cycling stability, therefore a potential fit to overcome the limits of vanadium dioxide when combined into a composite material. Nevertheless, rGO is plugged from restacking which lowers its specific capacitance. To fabricate a novel and excellent electrode material for high supercapacitor performances, an effective strategy was to dope the rGO with sulphur (S-rGO), which prevents the restacking and enhances its specific capacitance, before incorporating it into vanadium dioxide material. Thereby, vanadium dioxide sulphur-doped reduced graphene oxide (VO_2@S-rGO) composite materials were successfully prepared by a simple and rapid solvothermal process. The attained nanocomposite materials present good electron transfer and charge storage capacity/capacitance. Furthermore, the presence of sulphur revealed an increased pseudocapacitive behaviour and a good wettability at the electrode/electrolyte interface. An asymmetric device is fabricated using the optimized VO_2@S-rGO-1 composite and cocoa-derived activated carbon (Cocoa-AC) as positive and negative electrodes, respectively. The device exhibited specific energy and power of 32.6 W h kg^{-1} and 426.0 W kg^{-1}, respectively, in 0.5 M K_2SO_4 aqueous electrolyte at a specific current of 0.5 A g^{-1} within a cell voltage of 1.7 V.

Keywords: VO_2, sulphur-doped reduced graphene oxide, VO_2@S-rGO, composite material, asymmetric supercapacitor.

Stable Hybrid Supercapacitor Assembly with Nitrogen-Doped Graphene and Layered-Mxene (Ti_3C_2) Electrodes

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Effective disposal of spent supercapacitors at their end-of-life has been rarely addressed even withtheir emergence as the next generation storage technology to be used in renewable energy systems.These high-power, long cycle life devices with significant specific energy have been studied in a hybrid assembly using a 2D N-doped graphene synthesized (from a facile, low-cost graphite exfoliation in an aqueous salt electrolyte) and layered MXene nanostructures. The relatively low cost of electrochemical exfoliation makes commercialization and scale-up even more attractive. The asymmetric design exploited the merits of both electrode materials in a non-corrosive KNO3 electrolyte and exhibited noteworthy performance. The hybrid device could operate at a 1.6V voltage with remarkable stability, demonstrated by floating tests for > 3 days and cycling for up to 25,000 cycles. The outstanding stability combined with a specific energy of 28 W h kg-1 and amaximum power of 16 kW kg-1 offers exceptional device performance. This is elucidated to be linked to the dopants in the exfoliated graphene sheets and abundant reactive sites in the layered MXene nanostructure, that provides rapid ion transport dynamics and charge storage. The findingsof this work pave the path for designing safe and reliable energy storage devices using less toxic materials with comparable electrochemical performance to conventional supercapacitors.

Keywords: Electrochemical exfoliation, graphene, MXene, Neutral electrolyte, Supercapacitors

A Study of Porous Carbon Structures Derived from Composite of Cross-Linked Polymers and Reduced Graphene Oxide for Supercapacitor Applications

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In this work, cross-linked polymer-based porous carbonaceous materials were successfully synthesized through hydrothermal and chemical vapor deposition (CVD) methods. The as-prepared carbons were denoted as activated carbon from polyvinyl alcohol (AC-PVA), activated carbon from polyvinyl alcohol/reduced graphene (AC-PVA/rGO) and activated carbon from polyvinyl alcohol/reduced graphene/polyvinyl pyrrolidone (AC-PVA/rGO/PVP). The as-prepared samples' structural properties showed a higher degree amorphicity. The textural analysis displayed high specific surface areas along with high void fractions for the samples. The electrochemical analysis of the cross-linked polymer-based activated carbons conducted as three-electrodes revealed the samples' potential as electrode materials for supercapacitors' applications. Activated carbon from PVA/rGO/PVP exhibited a superior specific capacitance (223 F g^{-1}), a smaller charge transfer resistance (R_{CT} = 1.0 Ω) and equivalent series resistance (ESR = 0.54 Ω) as compared to AC-PVA and AC-PVA/rGO. The symmetric device (AC-PVA/rGO/PVP//AC-PVA/rGO/PVP) delivered a high specific energy of 19.5 W h kg^{-1} corresponding to a specific power of 400 W kg^{-1} at 0.5 A g^{-1}. Besides, the supercapacitor revealed a good coulombic efficiency of 99.8% and capacitance retention of 82.3% over 10 000 galvanostatic charge/discharge cycles at a cell potential of 1.6 V at 5.0 A g^{-1} in 2.5 mol L^{-1} KNO_3 aqueous electrolyte. These encouraging results demonstrate the versatile potential of the carbon materials for future electrochemical energy storage devices.

Keywords: Supercapacitor; Electrode; Polymer; Composite; Activation.



POSTER **PRESENTERS**

Structural Properties of Off-Stoichiometric Fe-Ti-Sn and Fe-V-Al Heusler Alloys

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Among a variety of thermoelectric materials, a considerable attention has been paid to the semiconducting Heusler alloys, which are ternary intermetallic compounds. The most actively studied in this respect materials are the Heusler alloys based on MNiSn and MCoSb (M = Ti, Zr, Hf) with a C1b type of crystal structure (so-called half-Heusler alloys) and Fe2YZ (Y = V, Ti; Z = Al, Sn) with a L21 type of crystal structure (so-called full-Heusler alloys). Stability of these compound is largely governed by the valence electrons count. Specifically, most of the existing half-Heusler alloys have 18 valence electrons (e.g., TiNiSn, TiCoSb) while most of the full-Heusler alloys have 24 valence electrons (e.g., Fe2VAl, Fe2TiSn).

It has been suggested recently [1] that single-phase half-Heusler compounds can be obtained from structurally unstable alloys having 19 valence electrons by introducing defects to adjust their valence electrons count (VEC) to 18. This idea has been found to be fruitful for the case of half-Heusler alloys [1]. In our work we extend this approach to the case of full-Heusler alloys. Specifically, we prepared off-stoichiometric Fe2VAl and Fe2TiSn full-Heusler alloys whose chemical composition was chosen in such a way to fulfil VEC = 18. Investigation of structural properties of the prepared alloys showed that the nominal VEC = 18 off-stoichiometric Fe-Ti-Sn is a multiphase compound while the off-stoichiometric Fe-V-Al exists as a single-phase compound. Structural instability of the off-stoichiometric Fe-Ti-Sn is most likely due to its specific phase diagram [2]. On the other hand, the existence of the single-phase off-stoichiometric Fe2VAl with nominal VEC = 18 opens up a new window for the desing of previously unknown thermoelectric Heusler alloys.

Keywords: Thermoelectrics; structure; Heusler alloys

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Plastic Waste: Fuel Conversion, Characterization and Life Cycle Analysis.

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The pyrolysis of plastic waste is a practical solution for plastic waste pollution in our environment here in Ghana, West Africa. Pyrolysis, which is decomposition brought about by high temperatures in the absence of oxygen, enables the conversion of polyethylene (PE) into liquid fuel and flammable gas. PE depolymerization started at around 150°C and propagated gradually until the temperature reached around 385°C - 410°C. After that, the temperature began to drop indicating the end of the pyrolysis process and liquid fuel, combustible gas and char were achieved. Acquired fuel was then analysed via FTIR, UV- VIS and GC-MS. These indicated the presence of aromatic compounds, alkenes and peaks of alkanes. With data collected (energy consumption inputs and outputs), the life cycle impact of the entire plastic waste pyrolysis process was calculated in openLCA software. This calculation exposed eighteen impact categories with human carcinogenic toxicity as the highest impact at 34% with a value of 0.0078kg 1,4-DCB and water consumption as the least at 0.0093% with 2.10351E-06m^3. The endpoint area of protection calculations was also recorded.

Keywords: Pyrolysis, fuel, polyethylene, characterization, impact

Activated Cashew Carbon-Manganese Oxide Based Electrodes for Supercapacitor Applications.

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The current global energy challenge which affects most developing countries in particular, is of major source of concern today. The availability of less expensive techniques of storing excess generated energy is critical to the success of the renewable energy roadmaps implementation. In this study, hydrothermal and chemical leaching methods have been used to synthesize MnO_2 nanoparticles using $KMnO_4$ and $MnSO_4$ as precursors at 140°C and from natural local manganese ore. Activated Carbon (ACF) have also been produced from agricultural Cashew biomass waste, through a physical carbonization and KOH activation process using temperatures of 700°C- 900°C for periods between 1-2 hours. The as-prepared materials have been characterized via XRD, Raman, FTIR, SEM. Electrochemical performance measurements (CV, EIS and GCD) were carried out on the prepared electrodes. The specific capacitance values obtained were in the range of 2.8F/g - 6.5F/g at different scan rates of 20mV -50mV respectively in a potential range of -0.4 to +0.4V and -0.4 to +0.6V for the various types of electrodes.

Keywords: Supercapacitor, Activated Carbon, Agrowaste, characterization, electrochemistry

Dopant-Free Polymeric Hole Transport Materials for Improved Performance of All-Inorganic Perovskite Inspired Solar Cells.

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Since lead toxicity and instability are a concern for lead halide perovskite, research has recently focused more on the development of lead-free and stable perovskite absorbers. All-inorganic cesium antimony iodide ($Cs_3Sb_2I_9$) perovskite inspired material (PIM) has recently gained considerable interest as an appropriate replacement for Pb-based perovskites. Herein, we describe $CS_3Sb_2I_9$ perovskite inspired solar cells employing different polymer hole transport materials such as 2,2′,7,7′-tetrakis-(N,Ndi-p-methoxyphenyl-amine)-9,9′-spirobifluorene (spiro-OMeTAD), poly(3-hexylthiophene-2,5-diyl) (P3HT), poly[[4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-b:4,5-b′]dithiophene-2,6-diyl][3-fluoro-2-[(2ethylhexyl)carbonyl]thieno[3,4-b]thiophenediyl]] (PTB7) and copper thiocyanate (CuSCN). One-step, antisolvent-free deposition method is employed in the deposition of $Cs_3Sb_2I_9$ perovskite inspired films with a final device architecture of TiO_2|$Cs_3Sb_2I_9$|HTM|Au. We comprehensively characterize the properties of the deposited $Cs_3Sb_2I_9$ PIM films by combining UV-visible (UV-Vis) absorption spectrum, photoluminescence (PL) spectrum, scanning electron microscope (SEM) and x-ray diffraction (XRD). Contact angle measurement is employed to examine the polar nature of the exposed surfaces utilizing different hole transport materials. The contact angles of the perovskite films with polymeric additives are much larger, revealing the hydrophobic nature of P3HT, P3HT and CuSCN (≈92 °) while spiro-OMeTAD show water contact angle ≈60 °. Solar cells prepared using PTB7 hole conducting materials exhibit substantially higher performance with PCE of 1.9 % compared to 1.4 % and 1.3 % for P3HT and CuSCN HTMs respectively. PTB7 and P3HT have revealed to be promising HTMs to produce higher performance and improved stability of such solar cells. Photocurrent conversion efficiency (PCE) of 2.0 % has been achieved for device utilizing spiro-OMeTAD hole selective material. However, the devices with spiro-OMeTAD HTM are highly unstable.

Keywords: All-inorganic perovskite solar cells, Polymeric HTMs, $Cs_3Sb_2I_9$, Antisolvent -free.

Wear Characteristics of TaN Reinforced TiAl-Based Composites

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Herein, the wear behaviour of 0, 2, 4, 6, 8, and 10 wt.% of TaN reinforced TiAl-based composites against Alumina balls were investigated under dry conditions. The wear features of the TiAl alloy were also examined as the reference material. The developed materials via spark plasma sintering process at a sintering pressure of 50 MPa, 100 °C/min, 1150 °C, and holding time of 10 mins were subjected to wear evaluation at different loads of 5 N and 10 N. The results indicated that TaN reinforcement enhanced the wear resistance of the TiAl matrix, which increases with increasing TaN addition. However, higher wear resistance was observed at a higher load of 10 N. The relationship between the wear attributes, such as surface roughness, morphologies, and composition, was evaluated.

Keywords: Titanium Aluminide, Sintering, Wear Resistance, Composites, Tantalum Nitride

Exploratory Study of Local Cassava Starch as a Green and Sustainable Polymer Binder for High-Performance Lithium-Ion Battery

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The commonly used binder in Lithium-Ion Batteries (LIBs) is a synthetic water-insoluble polyvinylidene fluoride (PVDF) polymer. It is typically dissolved in an environmentally toxic solvent such as N-methyl-2-pyrrolidone (NMP). The need to develop an aqueous-based binder (ABB) has dominated research publications for some time now. These include the application of water-soluble synthetic polymers such as polyvinylpyrrolidone (PVP), polyvinyl alcohol (PVA), polyacrylates, and water-soluble bio-degradable polymers such as carboxymethyl cellulose (CMC). The application of Man-made aqueous-based polymer in LIBs has the potential to reduce the environmental impact of LIB. The comparative life cycle assessment investigation of switching from NMP to ABB showed a drastic reduction in CO_2. More significantly, PVDF is considered teratogenic and mutagenic and NMP is regarded as a teratogenic, hazardous, and irritating compound. On the other hand, Ghana ranks among the top five (5) cassava producers in Africa with at least eighteen different improved varieties produced in commercial quantities for diverse industrial applications including starch production. Starch is the second most plentiful biomaterial in nature. It is eco-friendly because it is biodegradable, inexpensive, and readily available. In this preliminary study, local cassava starch is treated and prepared as a polymer binder for LIBs application. The binder is applied in Lithium nickel manganese cobalt oxides electrodes as a cathode in LIBs. At ambient temperature, the electrodes showed remarkable stable cycle performance at 1.0 C-rate compared to the electrodes made of PVDF. The electrodes displayed a discharge capacity of 144 mAh/g and 75 mAh/g for cassava starch and 140 mAh/g and 28 mAh/g for PVDF at 0.1 C-rate and 10 C-rate respectively. The superior electrochemical performance of the local cassava starch and its unique properties make it a potential alternative to the petroleum-based binder.

Mechanical Investigation of the Consolidated Particulate-Aluminium Matrix Composites

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Powder metallurgy processes allow the synthesis of materials with suitable dispersions at a relatively low cost. It entails blending different alloyed or pre-alloyed powders and fabricating the samples via various methods. The powder metallurgy route turns metallic powders into compacts via mechanical alloying and spark plasma sintering approach (SPS). In this study, dinickel boride particulate was mixed with aluminum matrix in a Turbula mixer to attain homogeneity of the powders. The consolidation was carried out in the spark plasma sintering machine using an optimized sintering parameter. The retrieved fabricated compacts were ground and characterized. Scanning electron microscopy was used to determine the sample morphology, and the samples' tensile properties and nanomechanical properties were evaluated. The outcome of the analysis showed that the particulates were distributed in the aluminum matrix, and as the particulates increased from 2 wt.% to 8 wt.%, some agglomerations were observed in the microstructures. The nanohardness and elastic modulus of the fabricated composites improved compared to the aluminum matrix due to the addition of the particulates. The tensile behavior of the fabricated composites demonstrated an improvement in the ultimate tensile strength at the expense of the elongation of the fabricated samples, possibly on account of load transfer from the matrix to the reinforcements.

Keywords: Dinickel boride; Aluminum; Tensile properties, Morphology, Nanomechanical properties.

Performance Evaluation of Solar-Assisted Heat Pump Dryer Integrated with Thermal Energy Storage for Drying *Moringa Oleifera* Leaves

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Plants used for medicinal purposes are extremely perishable, owing to moisture-enhanced enzymatic and microorganism activity, climate change, and improper handling and storage. Experiments have shown that drying the medicinal plant without affecting the bioactive nutrients and reducing the moisture content as much as possible can extend its shelf life. Different traditional and modern drying techniques for preserving medicinal plants have been developed, with some still being improved in Sub-Saharan Africa. However, many of these methods fail to address the most common issues encountered when drying medicinal plants, such as nutrient loss as a result of long drying times, and a limited capacity to dry during the evening or cloudy hours. Heat pump drying is an alternate drying method that results in no nutritional loss. Furthermore, combining a heat pump dryer with a solar energy storage system appears to be a viable option for all-weather drying without affecting the nutritional values of dried products. In this study, a solar-assisted heat pump dryer integrated with thermal energy storage is developed for drying *Moringa Oleifera* leaves. The study also discusses the performance analysis of the developed dryer as well as the proximate analysis of the dried *Moringa Oleifera* leaves. All experiments were conducted from 11 a.m. to 4 p.m. to assess the dryer's performance in “daytime mode”. Experiment results show that the drying time was significantly reduced, and the dryer demonstrated high performance in preserving all of the medicinal nutrients. In 5 hours of the drying process, the moisture content was reduced from 75.7 to 3.3%. The average COP value was 3.36, confirming the dryer's low energy consumption. The findings also revealed that after drying, the content of protein, carbohydrates, fats, fiber, and ash greatly increased.

Keywords: heat pump dryer; thermal energy storage; performance; moringa leaves; proximate analysis

Understanding Aluminium Graphite Dual-Ion Batteries: Device Configuration and Interface Evolution

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Aluminium batteries have emerged as a promising post-lithium energy storage technology with high power density (3000W/kg), high raw material abundance, and the opportunity for efficient end-of-life recycling [1-2]. Consisting of an aluminium metal anode, a graphitic carbon cathode and an ionic liquid electrolyte, AGDIBs operate by electrodeposition/dissolution of aluminium at the anode and intercalation/deintercalation of chloroaluminate anions at the cathode during charge/discharge [3]. However, AGDIB development is held back by a lack of fundamental understanding, particularly of the processes at the electrode-electrolyte interfaces. The acidic electrolyte, while non-flammable, poses challenges of corrosion which affect all cell components [4-5]. Especially the processes of corrosion, oxide evolution, and dendrite formation at the anode surface are not yet well understood. Motivated by promising results on an optimised graphene nanoplatelet cathode and $AlCl_3$-trimethylamine hydrochloride electrolyte [6], this work aims to complete understanding of the device by studying the aluminium anode surface and the impact of device configuration. Assembly procedures were explored with a focus on corrosion, material composition, and pressure, revealing the importance of aluminium purity and the limitations of molybdenum in inhibiting corrosion. Detailed surface characterisation was used to investigate anode-electrolyte interface evolution. Time of flight secondary ion mass spectrometry (ToF-SIMS) and x-ray photoelectron spectroscopy (XPS), complimented by optical microscopy and scanning electron microscopy (SEM), were used to probe the composition of an oxide layer and indicate that chlorine and iron are incorporated into the oxide during cycling. Depth profiling was used to deconvolute how the presence of different compounds impacts the formation of other species in this interphase layer. This work reveals that the evolution of the anode-electrolyte interface is more complex than previously assumed, and how careful consideration of device architecture can play a significant role in optimising this crucial phenomenon and improve device performance.

Keywords: aluminium graphite dual-ion battery, aluminium anode, aluminium oxide film, ionic liquid, corrosion

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Templated Carbon Films Vs. Conventional Catalyst Particles with FeN4 Sites for Oxygen Reduction in Gas-Diffusion-Electrodes

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In the search for alternative catalysts for the oxygen reduction reaction (ORR) at the cathode in fuel cells to substitute expensive platinum (Pt), atomically dispersed iron sites coordinated to nitrogen in a carbonaceous material (Fe-N-C) emerged in the last decade. Preparation protocols to maximize the site density usually rely on a two-step protocol, in which carbon-nitrogen precursors are pyrolyzed at high temperatures and iron is adsorbed in a second step into suitable nitrogen-coordinating host sites. (1,2) Despite the progress in iron content, high loading catalyst layers are required to be able compete with Pt catalyst layers in fuel cells. The resulting thick catalyst layers face mass transport issues at high current densities. (3) Freestanding catalyst films, whose porosity is controlled across the entire thickness of the catalyst layer might improve the mass transport at high current densities. Mesophase pitch-based films have been templated by silica (SiO2) nanoparticles (4), which have to be etched under time-consuming and harsh conditions. In our work, SiO2 nanoparticles are substituted by polystyrene nanoparticles, which decompose and tracelessly evaporate during the carbonization process. In contrast to the 12 micrometer thick films, which have been loaded with Pt, the thickness of the films is increased to 80 µm, which is common in Fe-N-C-based cathodes. Iron phthalocyanine (FePc) as a model active site is adsorbed on the freestanding carbon film. Gas-Diffusion-Electrodes (GDE) are appropriate setups to study such freestanding thin film catalysts. (5) A comparison of the ORR performance of catalyst layers, based on carbon films support (A) and conventional carbon particle support (B) with same FePc loading are presented.

Keywords- Templated Carbon Films, Freestanding Catalyst Films, Oxygen Reduction Reaction, Gas-Diffusion-Electrodes, Sustainable Energy Materials

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Elaboration and Photovoltaic Characterization of Nanostructures of Silicon

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With energy being a vital global issue, research in the field of photovoltaics continues to grow. Silicon photovoltaic cells dominate the world market. One of the reasons that limit the efficiency of silicon-based solar cells are the losses due to thermalization, so new concepts based on the development of new materials consisting of nanometric layers that could eventually allow to achieve efficiencies of 25 to 30%. The objective of this work is to develop silicon nanowires by a simple and inexpensive method for improving the efficiency of silicon-based photovoltaic cells. For this purpose, we have fabricated silicon nanostructures by the Metal Assisted Chemical Etching (MACE) method. The results obtained from Scanning Electron Microscopy (SEM) reveal very porous nanotexture that were observed on the silicon surface. The nanostructuring is followed by a doping with a Phosphorus Oxide (P2O5) based gel using the sol-gel thin film deposition method (spin caoting) and a thermal annealing for the diffusion of phosphorus in a very deep and homogeneous way on the whole silicon surface. The currentvoltage characterization of silicon nanowire cells obtained under different etching times allowed us to determine the photovoltaic parameters. For the nanowires obtained at etch times of 30, 45 and 60 min we have respectively yields of 17.32%, 16.66% and 14.59%. For the samples that are etched under light their yields give 22.90%, 21, 33% and 25.53%.

Keywords: characterization, doping, etching, MACE, nanostructures, nanowires, photovoltaic cells, silicon

Assymetric Birnerssite-Type Mno_2-CNT and Nanostructured AC Device for Supercapacitor Application

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MnO_2-CNT synthesized via facile hydrothermal reflux technique and nanostructured activated carbon prepared via chemical impregnation and carbonization with excellent morphological and electrochemical properties are reported in this work. The material device tested in 1M $LiSO_4$ aqueous electrolyte displayed a good energy density at a current density of 0.5 A/g with a maximum 2V working potential. The device showed good potential for supercapacitor application.

Key words: MnO_2, CNT, Activated carbon, hydrothermal, supercapacitor

N-I-P Perovskite Solar Cell Design Optimization for High Efficiency using SCAPS-1D

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p-i-n structures are gaining popularity in organic-inorganic lead halide perovskite solar cell (PSC) research due to their more straightforward fabrication method and low-temperature fabrication process for flexible and tandem systems compared to an n-i-p structure. In this study, six n-i-p perovskite architectures and a tandem cell were simulated to maximize the power conversion efficiencies by varying the thickness of the layers using Solar Cell Capacitance Simulator (SCAPs 1D). All-metal oxide transport layers comprising of three different electron transport materials (ETM), TiO_2 (the most common for mesoscopic and n-i-p structures), ZnO and PCBM, are explored with the hole transport material (HTM), NiOx and CuSCN. A PSC structure based on Methyl Ammonium Lead Iodide, CH3NH3PbI3, was employed for the absorption layer. Detailed analyses were conducted for open circuit voltage (Voc), short circuit current (Jsc), fill factor (FF), and power conversion efficiency (PCE), taking into account the fluctuation of perovskite layer thickness, ETM and HTM thickness, and Temperature difference. According to findings, the best absorber thickness for the perovskite layer was 745 nm, and an ETM, ZnO, has been demonstrated to be more effective than TiO_2. Furthermore, due to greater carrier mobility and optical absorption, ZnO exhibits superior PCE and Jsc in nearly all circumstances. Furthermore, our investigation determined that ZnO and PCMB are slightly less sensitive than TiO_2. Finally, tandem solar cells surpass all other researched cell types in terms of power conversion efficiency. The tandem cell attained a combined PCE of 40.10%. Thus, this work presents a comprehensive investigation of the effect of interfacial layer features on the performance of different n-i-p PSC.

Keywords: Organometal halide perovskites, Absorption Layer, Hole Transport Materials, Electron Transport

Repurposing 18650 Cylindrical Lithium-ion Battery for a Second Life - Feasibility and Environmental Impact in Solar Photovoltaic Microgrid Applications

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Projection of global lithium battery demand indicates a 14-fold increase in the use of batteries in consumer electronics, energy storage systems, and electric vehicles between 2018 and 2030. (Haram et al., 2021). Electronic waste from these batteries nearing the end of their useful lives is already a global problem, with more severe consequences in several African and Asian countries that lack formal recycling facilities. As a result, these lithium-ion batteries are dumped in landfills, where informal recyclers collect, dismantle, and crudely process them by hand to reclaim their valuable but toxic metals (e.g., cobalt). These informal processes endanger public health, safety, and the environment. This study examines the viability of cascading 18650 cylindrical lithium-ion cells, which were collected from electronic hubs in and around Lagos, Nigeria, and are nearing the end of their first life in consumer electronics, for a second life as Stationary Battery Energy Storage Systems for use in Solar Photovoltaic Microgrids. Using the Homer Pro Software, it also compares the cost per kWh and direct carbon emissions of first-life battery energy storage systems and diesel power generation. Exploring a circular economy perspective for the lithium battery life cycle.

Keywords: Circular Economy, Second Life Battery Energy Storage Systems (SLBESS), Stationary Battery Energy Storage Systems, Solar Photovoltaics, Microgrids

Bamboo-based Activated Carbon as Electrode Materials for High Supercapacitor Performance

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Synthesis of activated carbon (AC) from biomass has recently become one of the main focus for the majority of the scientific community. In this study, activated carbon derived from bamboo stem was explored as potential materials for energy storage applications. Activated carbon were synthesized via chemical vapor deposition process at different temperature through Argon gas flow. The synthesized samples were firstly characterized using X-ray fluorescence spectroscopy (XRF). XRD, Raman spectroscopy SEM, and TEM will be examined to further investigate the as-prepared materials. The electrochemical properties were evaluated by cyclic voltammetry (CV), galvanostatic charge/discharge (GCD), electrochemical impedance spectroscopy (EIS) and cycling stability tests in three-electrode configuration using 6 M KOH aqueous electrolyte within a potential window range of 0.0 - 0,75 V. The sample synthesized at 850 °C showed a superior specific capacitance of 169.7 F g^{-1} at a specific current of 1 A g^{-1}. The cycling stability test recorded a capacitance retention of 92.2% up to 10,000 galvanostatic charge/discharge at 10 A g^{-1}. The synthesized materials showed promising properties as electrode materials for high performances supercapacitor applications.

Keywords: Bamboo, activated carbon, electrode material, supercapacitor, energy storage

Design of Novel Electrochemical Reactor Derived from Cobalt Phosphide and Biomass as composite materials for Green Hydrogen Production from Water

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Hydrogen is a promising renewable energy carrier to replace fossil fuels due to its zero emissions, and high energy density (~ 142 MJ/kg) which can be used in conjunction with renewable energies that are intermittent. The objective is to find an alternative to noble metals such as Ir, Ru, Pt, Ti which can provide a current density superior to 2 A cm^{-2} and an important efficiency up to 84%. In this study carbon cobalt phosphide ($C_oP@C$) will be synthesized using extract from biomass peanut shell waste as carbon source, cobalt nitrate hexahydrate and sodium hypophosphite monohydrate as cobalt and phosphorus sources, respectively. The synthesized composite materials, $C_oP@C$ will be used as a catalytic electrode for the hydrogen evolution reaction HER. The first prepared materials by adopting a hydrothermal approach were examined using X-ray photoelectron spectroscopy (XPS), which revealed cobalt phosphate octahydrate ($Co_3(PO_4)_2.8H_2O$) composite material. The obtained $Co_3(PO_4)_2.8H_2O$ samples were explored as electrode material for supercapacitors applications using 6 M KOH aqueous electrolyte in three-electrode configuration. The electrode delivered a specific capacity of 54 mA h g^{-1} at a specific current of 0,5 A. g^{-1} within a potential window range of 0.0 – 0.5 V. It showed good stability with a coulombic efficiency of 100% up to 7000 galvanostatic charge/discharge cycles at 10 A g^{-1}. Other characterizations techniques will be investigated. The synthesis of $C_oP@C$ will be carried out via low cost and efficient strategy to effectively address the challenge of the energy.

Keywords: hydrogen, current densities, efficiency, cobalt phosphide, biomass, energy

Development and characterization of spinel-based composite materials ($MnCo_2O_4$@g-C_3N_4/C60) from peanut shell wastes extracts for electrochemical capacitors

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In this work, we incorporate carbon-based materials such as fullerene (C60) and graphitic carbon nitride (g-C_3N_4) in manganese cobalt oxide ($MnCo_2O_4$) matrix via a green synthesis method for supercapacitor applications. The $MnCo_2O_4$ @ C60/g-C_3N_4 composite was synthesized through a green solvothermal method from an aqueous extract of *Arachis hypogaea* biomass (peanut shell) as solvent. Different times were investigated to optimise the samples (2h, 4h, 8h, and 16h).

The structural and morphological properties as well as the chemical composition of the composite samples were evaluated using Raman spectroscopy, X-ray diffraction (XRD), scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS). The results show that this composite contains graphitic carbon nitride and C60 carbon originating from the peanut shell.

The electrochemical properties were evaluated by cyclic voltammetry (CV), galvanostatic charge/discharge (GCD), electrochemical impedance spectroscopy (EIS), and stability tests (cycling and floating) in the three-electrode configuration using an aqueous basic electrolyte namely potassium hydroxide (KOH) with a concentration of 6 M under a potential of 0.5 V.

The results obtained in this study, in particular those of 8h sample which has a specific capacity of 20.1 mA h g^{-1} and a capacity retention of 69.6 %, show that this material is a promising candidate in the supercapacitor applications as a cathode.

Keywords: Green synthesis, Carbon-based Material, Composite, Peanut Shell, Cobalt Manganese Oxide, Supercapacitor.

Study of the Physicochemical Properties of Composite Materials Based on Nickel Oxide and Graphitic Carbon Using Cashew Leaf Extracts for Supercapacitor Applications

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Nickel oxide has been considered as a potential candidate for supercapacitor (SC) applications however, it remains a challenge for improving the low lifetime and poor electrical conductivity. Carbon-based materials pocess high specific surface area and good electrical conductivity as well as excellente cycling stability and then a great fit to overcome the nickel oxide drawback. Carbon materials play an important role in supporting pseudocapacitive and Faradaic materials. Thereby, composite from carbon-based and pseudocapacitive materials can provide excellent supercapacitors properties by combining the merits of each component. Biomass-derived carbons (BDCs) are excellent materials for electrochemical capacitors due to their important characteristics, such as durability, renewability specialy their abundant nature and low cost.

In this work, composite materials of NiO and biomass-derived carbon (BDC) were prepared by a hydrothermal process using cashew leaf extract and nickel nitrate hexahydrate as precursors. The X-ray diffraction (XRD) spectrum indicates the presence of NiO. SEM, XPS, EDX and Raman spectroscopy will be investigated to identify the nature and morphology of the samples. Electrochemical tests will be performed to evaluate the performances of the composite materials as electrode for SCs applications.

Keywords: NiO, graphitic carbon, composite materials, supercapacitor, energy storage

Impact of the gamma-ray irradiation on the microstructure of vanadium dioxide layers as intelligent coatings for passive energy management

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Vanadium dioxide has significant thermochromic properties, reversible Metal Insulator Phase Transition (MIT), lowest transition temperature (Tt) at 68 °C, good thermal stability, drastic change in its IR transmittance then, a good candidate for <<intelligent>> passive energy coating management. The development of micro and picosatellites requires new devices for the protection of the spacecraft against temperature variations, depending on the satellite in orbit, either it is exposed to the sun or is in the shadow of the earth. These new devices do not meet the mass, surface and electrical power requirements of miniature satellites. A passive thermochromic device such as the VO_2 could provide this protective function. However, for an efficient use of this type of coating in the space domain, it is essential to study the impact of gamma irradiation on the high crystalline quality and the optical properties of VO_2. The nanostructured thin films are not modified and the material has a good crystalline quality with a monoclinic phase structure. While the phase transition is complete at this temperature, this indicates that the irradiation dose does not influence the transition of these samples. Furthermore the microstructure is modified with a slight variation of the structure. In order to understand the mechanism that governs this modification, the evolution of the crystallites size on the (100) and (011) growth planes is evaluated.

Keywords: thin film, vanadium dioxide, crystallite seeds, microstructure, smart coatings.

Study of Thermal and Rheological Properties of Nanofluids Based on Iron Oxide Fe_2O_3

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Low thermal conductivity is a primary limitation in the development of energy-efficient heat transfer fluids that are required in many industrial applications. In this work, we propose an innovative new class of heat transfer fluids which can be engineered by suspending metallic nanoparticles in conventional heat transfer fluids. The resulting nanofluids are expected to exhibit high thermal conductivities compared to those of currently used heat transfer fluids, and they represent the best hope for an enhancement of heat transfer. The results of a theoretical study of the thermal conductivity of nanofluids with copper nanophase materials are studied. The potential benefits of the fluids are estimated, and it is shown that one of the benefits of nanofluids will be the dramatic reduction in heat exchanger pumping power.

Keywords: Iron oxide, nanoparticles, thermal energy

Development of composite materials based on VO_2 and C60 using extracts of Western cashew leaves for supercapacitor applications

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Carbon vanadium dioxide (VO_2)@C60 and carbon vanadium carbide vanadium dioxide (VO_2)@C60/VC were successfully synthesized from biomass leaves via a simple solvothermal method. Vanadium dioxide and vanadium carbide (VC) powder was added into the dry leaves of the western cashew tree solution, by a variation of the vanadium carbide mass (0,25g, 0,5g and 0,75g) incorporated different composites were obtained. The prepared materials were characterized by XRD, SEM, XPS and Raman spectroscopy. The addition of VC to the base material led to a significant improvement in electrochemical performance. The electrochemical properties evaluated in three-electrode configuration exhibited a specific capacity of 7.44 $mA.h.g^{-1}$ for VO_2(B)@C60 sample while the optimized composite VO_2(B)@C60/VC displayed a specific capacity of 34.95 $mA.h.g^{-1}$ at a specific current of 0.5 $A.g^{-1}$ within a stable potential window ranging between 0.0 to 0.5 volts. The optimized composite showed a capacity retention of 32% at 10 A g^{-1}. The VO_2(B)@C60/VC (0.5g VC) electrode material proved better performance as-compared to VO_2@C60, VO_2(B)@C60/VC (0.25g VC) and VO_2(B)@C60/VC (0.75g VC) electrodes which have specific capacities equal to 7.44 $mA\ h.g^{-1}$, 8.456 $mAh.g^{-1}$ and 26.16 $mA.h.g^{-1}$ respectively. Overall, VO_2(B)@C60/VC (0.5g VC) composite material is a promising electrode for practical supercapacitor applications due to the good electrochemical performance, rapid and easy preparation.

Keywords: Green synthesis, Vanadium dioxide, Carbon-based materials, Western cashew tree, Supercapacitors

Optimization of The Amount of Ferroelectric Inorganic Perovskite Nanoparticles for High Efficiency Indoor Photovoltaic Cells

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In the search for higher efficiency, perovskite solar cells are the focus of attention in the photovoltaic community. Compared to other technologies (amorphous silicon (a-Si), organic photovoltaics (OPV), dye-
sensitized solar cells (DSSC)), perovskite-based solar cells have an efficiency of more than 25% during a
record time of 5 years [1]. On the other hand, these types of cells have shown excellent efficiencies in recent years when exposed to low light, with records of around 40% [2]. However, these materials have a real problem with the stability of their performance over time and under extreme conditions. They also have the misfortune of containing lead in their formulation. One solution seems to be the use of other types of perovskites such as ferroelectric ones. Ferroelectric perovskite such as PZN-4.5PT is a promising material offering high performance and low cost for indoor application. Thus, in this work, we developed organic-inorganic hybrid solar cells with perovskite nanoparticles dispersed in a biopolymer. The amount of nanoparticles was optimised for a more efficient performance. I-V measurements showed, for a 2.4 cm2 cell on ITO substrate, an efficiency of 30% at an irradiance of 1092.71 Lux with a very high open circuit voltage VOC, a short circuit current of 1.61.10-4 A and a form factor FF of 0.46. Apart from the use of
Ferrophotovoltaic perovskites, the use of local plant-based molecules as a matrix and charge transport material had a real impact on this performance and could be safe to reduce the adverse environmental effects with the low number of perovskites used.

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Keywords: Perovskites, ferroelectric, nanoparticles, biopolymer, thin film.



SYMPOSIUM-04
MATERIALS FOR WATER & ENVIRONMENT MONITORING



KEYNOTE SPEAKERS



Martin Thuo is a Professor in the Departments of materials science & engineering at North Carolina state University. Prior to NCSU, he was a faculty at Iowa State University in the department of Materials science and engineering and electrical & computer engineering. He was a Mary-Fieser (2009-2011) and NSEC (2011-2013) Fellow at Harvard University under Prof. George M. Whitesides. He is the recipient of several awards like the ACS nano rising star, Akinc excellence in research award, Schafer 2050 professorship, Lynn-Anderson research excellence award, Black & Veatch faculty fellowship, among others. His research interests encompass the general theme of surface thermodynamics for frugal innovation through simplicity.

Frugal Engineering: from Heat-Free Solders, Tunable Bandgaps, to Low-Cost Diagnostics

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Need for flexible/wearable electronics, post-CMOS electronics, or ultra-miniaturization of hybrid microelectronics, calls for low temperature and autonomous (self-assembly) fabrication. Concomitant need for energy efficiency during and post manufacturing exacerbates these challenges. We couple fundamental surface thermodynamics and bottom-up self-assembly to design material synthesis and processing approaches that can meet these demands. This talk discusses the nature of metal nanointerfaces (<10 nm) and how felicitous choice of processing approaches lead to surface/interface-driven tuning of the thermodynamic energy landscape of the material. This altered landscape enables frugal low energy manipulation of the material by driving relaxation or reactions via low energy pathways. Surface-directed navigation of the energy landscape manifests as metastable states (specifically undercooling), surface composition inversion (chameleon and hedgehog-like surfaces), inverted (inside-out) thermal degradation to create graphene/graphene oxide macrotubes, and surface plasticity or amphiphobicity for size-controlled feature formation or wetting. We will explore how these breakthroughs are; i) advancing micro- or printed- electronics manufacturing, ii) enabling synthesis of high aspect-ratio synthons of electronic materials through *ad infinitum* polymerization, iii) translation of these hybrid electronic materials synthons into self-assembled diodes and gates, and iv) albeit briefly, we'll demonstrate how these principles in surface/interface engineering can be expanded to other areas like controlled wetting for affordable diagnostics.



Dr. Sergi Garcia-Segura *is currently an Assistant Professor at Arizona State University. He holds a B.S. degree in Chemistry from the University of Barcelona and a B.S. degree in Material Science Engineering from the Polytechnic University of Catalonia. He conducted a M.S. in electrochemistry science and engineering at the University of Alicante and completed his Ph.D. in Physical Chemistry at the University of Barcelona.*

Dr. Garcia-Segura research seeks to develop sustainable water treatment technologies by using nano-enabled photo-assisted and electrochemically driven catalytic processes. He has worked across four continents in multidisciplinary teams, aiming to ensure availability and sustainable management of water and sanitation for all. His contributions to the field of environmental electrochemistry (> 140 articles with h= 52) have been recognized by international awards including the Environmental Electrochemistry Prize of the International Society of Electrochemistry, the Green Talent Award from the German Federal Ministry of Education and Research, and the Elsevier-International Society of Electrochemistry Prize for Applied Electrochemistry. Recently he has been highlighted as Rising Star in Science 2022. He is an editor of Chemosphere (Elsevier) and Water Science & Technology (IWA).

Enabling Decentralized Electrochemical Water Treatment in The Nexus with Materials Science

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The United Nations has identified water and sanitation as one of the sustainable development goals (SDG) to reach by 2030. However, we are running against time to reach such idealistic goal. At least 129 countries may not reach the goal of having sustainable managed water by 2030. Figure 1 illustrates the percentage of global population that still lack access to clean drinking water and safely managed sanitation.

Conventional water treatment systems rely on centralized water treatment plants that ensure water quality standards before distributing the treated water via dedicated distribution networks. Such traditional approach lays on the premise of a high infrastructure investment that requires long term maintenance of a grid or distribution system, which may not be in place in many locations. In this context, decentralized technologies appear as promising solution to accelerate the pace towards reaching this sustainable development goal. Decentralized technologies should be modular, adaptable to different water needs, and user friendly to be operated by untrained personnel. In this frame, electrified processes that exploit unique electrocatalytic properties of charged interfaces arise as competitive approach.

This keynote presentation will describe fundamental aspects of electrochemically-driven technologies with emphasis on the relevance of electrocatalyst material selection and material engineering. Different challenges and research opportunities will be identified during the presentation through different case scenarios that exploit electrochemical technologies for decentralized treatment. Examples of modular units based on electrochemical advanced oxidation processes, electrochemical advanced reduction processes, and electrodisinfection will be used to showcase competitiveness of electrified water treatment at different scales. The discussion will be sustained using techno-economic analysis to assess cost-competitiveness.

Keywords: Electrocatalysis, material-light interaction, water treatment, disinfection



Elisa Moretti *is Associate Professor of Inorganic Chemistry at the Department of Molecular Sciences and Nanosystems, Ca' Foscari University of Venice (Italy). After receiving a PhD Degree in Chemistry at the Ca' Foscari University, she spent several research periods at the University of Malaga (Spain) and the Institute of Materials Science CSIC-University of Seville (Spain) for a post-doctoral experience. She is leading a multidisciplinary group focusing on the development of advanced 0-3D nanostructured inorganic materials for energy and environmental applications (e.g. photocatalysis and electrocatalysis for* H_2 *production and purification, dyes and drugs photodegradation for water remediation, water desalination). EM is also co-founder and scientific supervisor of the Spinoff ChEERS srl - Circular Economy for Energy Recycling Solutions, for a sustainable upcycling and valorization of industrial and agri-food wastes.*

Design of Photoactive Multi-Component Nanosystems for Energy and Environmental Applications

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Nowadays, one of the main technological challenges that we are facing is the ability to provide a sustainable supply of clean energy and, among all renewable sources, solar energy displays the greatest potential. Recently, the development of novel synthetic strategies has led to the preparation of nanostructured materials displaying unique properties compared to the bulk counterpart systems, with controlled and tunable morphologies able to enhance the activity and selectivity of a heterogenous process.

This talk will focus on the importance of tuning the morphological features of a catalyst as a strategy to improve its photoactivity, focusing on how rationally designing inorganic materials at the nanoscale can lead to shapes and structures suitable to enhance the performance of industrially and environmentally important processes. The talk will discuss some energy and environmental applications that can be addressed by multi-component systems synthesized via the bottom–up approach, highlighting their structure-reactivity relationship. Photocatalytic H_2 production and purification, and drugs degradation will be presented as successful cases history



EARLY CAREERS- SPEAKERS



Dr. Bridget Mutuma *is a Research Associate Fellow at the Department of Chemistry, University of Nairobi, Kenya. She is an ARISE fellow (2022), AAS Affiliate (2021-2025), and an ASLP Fellow (2021). She has a BSc. degree in Analytical Chemistry from Kenyatta University, (Kenya, 2009), an MSc degree in Material Science and Engineering from Kangwon National University (South Korea, 2013) and a PhD in Chemistry from the University of Witwatersrand (South Africa, 2016). Dr Mutuma has extensive postdoctoral experience in nanomaterials, sensor technology and energy storage systems. Her research interest is on the development of core-shell nanostructures/carbon-based nanomaterials and their application in gas sensors, solar cells, supercapacitors and photocatalysis. In particular, she has pioneered research in the design and use of hollow carbons as gas-sensing materials. Her research findings have been published in over 30 peer-reviewed articles and presented at several national and international conferences. In the last few years, she has mentored and co-supervised BSc Honours, MSc and PhD students in the area of nanotechnology and materials chemistry. Dr Mutuma has been a member of the India-Brazil-South Africa (IBSA); Solar energy project, South African Chemical Society, and is a registered Professional Natural Scientist (Pr.Sci.Nat). Due to her research achievements, she has received several awards and fellowships; ACS PITTCON travel grant (USA, 2020), CNPq Visiting PhD Research Fellowship (Brazil, 2016), Penny Huddle Memorial Award (Witwatersrand University, 2015) and the Korean Government Scholarship Award (South Korea, 2010), among others.*

Valorization of Biodigestor Plant Waste in Electrodes for Supercapacitors and Microbial Fuel Cells

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Porous carbons are receiving great attention by scientists due to their tunable physicochemical and textural properties. In this work, lignin was activated with potassium bicarbonate ($KHCO_3$) in order to generate porous carbons via a one-step carbonization route. The lignin-to-$KHCO_3$ ratio affects the performance both in supercapacitors and oxygen reduction reaction (ORR) electrocatalysis. The lignin-derived carbons obtained at lignin/$KHCO_3$ mass ratios of 1:0.5 (LAC-0.5) and 1:2 (LAC-2) comprised of mesopores and micropores displaying BETs of 1558 m^2g^{-1} and 1879 m^2g^{-1}, respectively. LAC-2 electrode material exhibited a superior specific capacitance in 2.5 M KNO_3 electrolyte. A symmetric supercapacitor with LAC-2 electrodes was built displaying a specific capacitance of 28.5 F g^{-1}. This value corresponds to an electrode specific capacitance of 114 F g^{-1} and a specific energy of 10 Wh kg^{-1} with a corresponding specific power of 397 W kg^{-1}. Durability tests showed that the device was able to maintain a capacitance retention of 84.5% after 15,000 charge-discharge cycles. The lignin-derived carbons were also studied as electrocatalysts for ORR in a neutral medium. The LAC-2 showed higher electrocatalytic activity and superior ORR performance than LAC-0.5. The interconnected porous network and the high surface area made the lignin-derived porous carbons suitable electrode materials for dual applications.



Dr. Abdoulaye Thiam *is a researcher and professor in the Institutional Program for Promotion of Research, Development, and Innovation (PIDi) at the Metropolitan University of Technology (UTEM, Chile). Before joining PIDi-UTEM, Dr. Thiam was a postdoctoral researcher at the faculty of chemistry and biology at the University of Santiago, Chile. Dr. Thiam conducted his Ph.D. (within the Spanish interuniversity excellence program 'Electrochemistry: Science and Technology') under the supervision of Profs. Enric Brillas and Ignasi Sirés at the LEMMA (Laboratory of Electrochemistry of Materials and Environment, Faculty of Chemistry) in the University of Barcelona (Spain). Dr. Thiam main research has focused on the study of electrochemical advanced oxidation processes and the development and optimization of sustainable electrochemical technologies for water remediation. Dr. Thiam's group studies also the development and synthesis of news 2D and 3D nanoparticles with photocatalytic properties for the elimination of emerging contaminants using UV light or solar energy and electrochemical technologies.*

In 2017, he is awarded ISE-Elsevier Prize for Green Electrochemistry (International society of electrochemistry) for his works on electrochemical advanced oxidation processes, especially on Fenton-based processes.

Magnetic Nanomaterials as Sustainable Catalyst for Electrochemical Wastewater Treatment: A Cleaner Approach Toward Water Remediation

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Water and energy have a huge significance in determining people's economic and socialwell-being. Nowadays, the world is facing water supply and security threat due to massive industrialization, widespread urbanization, and lack of awareness among people toconsider water as a crucial commodity. During the last two decades, climate change causing extreme heat coupled with the decrease of precipitation rates have resulted in a chronic water deficit. Additionally, anthropogenic activities are leading to a diversity of new stable chemical contaminants in the environment that represents a major concern forwater management. Solving tomorrow's water issues is going to require innovative new approaches that include the development of micropollutants transformation technologiesto secure water quality.

Advanced oxidation processes (AOPs) offer practical solutions to remove emerging contaminants and enable water reuse strategies for water conservation. AOPs are chemical/photochemical methods based on the in-situ generation of highly reactive oxygen species (ROS) such as hydroxyl radical ($^{\bullet}OH$) (E^{o} = 2.8 V/SHE). Among AOPs,Fenton-based electrochemical AOPs and photocatalysis have generated great interest dueto the easy, clean, and effective way to produce oxidants. The main advantage of these processes over conventional ones is the environmental compatibility and the no requirement of chemicals addition as the main reagent is electron, which is an inbuilt clean species. However, its application at industrial level presents some important drawbacks. The recent use of heterogeneous catalyst such as natural and synthetic metal-based materials allowed to overcome these limitations.

This work presents an overview of electrochemical advanced oxidation processes and therecent development of novel hybrid photo-assisted electrochemical/photocatalysis process using recoverable magnetic nanomaterials as sustainable catalyst. Magneticnanomaterials based on iron nanoparticles, metal organic frameworks and graphitic materials such as MIL-100(Fe)@$CuFe_2O_4$, MIL-100(Fe @α-Fe_2O_3, g-C_3N_4 @$CuFe_2O_4$ or g-C_3N_4@α-Fe_2O_3 was synthetized and used as photoactive catalyst in the hybrid photoelectro-Fenton/photocatalysis process for the effective degradation of emerging contaminants. The morphology, crystal structure, chemical composition and magnetism were determined by SEM, TEM, XPS, FT-IR, XRD and vibrating sample magnetometer.By virtue of magnetic property, an external magnetic field is used for the effective separation of catalyst after treatment and reuse for other treatments.

Keywords: Wastewater treatment, emerging contaminants, electrochemistry, hydroxyl radical.



El Hadji Mamour Sakho, Ph.D.

Postdoctoral Fellow: University of Dakar, LPQEN Laboratory. I received my PhD degree in Applied Physics from Mahatma Gandhi University, India in 2016. I did four years of postdoctoral research in the Department of Chemical Sciences, University of Johannesburg, South Africa. I am currently a Postdoctoral Fellow at University of Dakar, LPQEN Laboratory. My research interests are synthesis and characterization of nanomaterial for different applications which include solar cells, batteries, nonlinear optical applications, sensor, photocalysis and polymer nanocomposites. In my current project, we develop green preparation of carbon/nanoparticles for supercapacitors application. In this project carbon materials are prepared from organic biomass and in situ decorated with noble nanoparticles such silver, copper, and gold as supercapacitor materials for clean and renewable energy storage.

Dye Adsorption Properties of Luminescent-Superparamagnetic MFe_2O4 (M = Mn, Mg)/Reduced Graphene Oxide Composites

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MFe_2O_4 (M = Mn, Mg)/reduced graphene oxide (MFe_2O_4/RGO) nanocomposites were synthesized through a simple and novel pressure cooker assisted solvothermal method. The nanocomposites were characterized using x-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), UV‑Vis absorption and photoluminescence spectroscopy, transmission electron microscopy (TEM) and x-ray photoelectron spectroscopy (XPS). The optical analyses showed that, the MFe_2O_4/RGO materials have good photoluminescence (PL) with excitation dependent PL properties while magnetic characterization indicated that, the as-synthesized MFe_2O_4/ RGO nanocomposites exhibits superparamagnetic behavior. The study on methyl blue (MB) dye adsorption revealed that, the as-prepared nanocomposites have strong and recyclable adsorption for MB.

Keywords: Synthesis, Luminescence; Superparamagnetic; Dye adsorption



INVITED SPEAKERS

Nanotechnology for Sustainable Water Treatment

ABDULKAREEM AMBALI SAKA

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Water is an essential resource needed on a daily basis for human consumption and usage. This resource is abundant on the Earth, covering over 70 per cent of the surface. Presently, the demand for clean and affordable water has already exceeds the supply. Due to this growing demand in supply of quality water, the growth of the health, industrial and economic sector have been grossly affected. According to United Nation Education Science and Cultural Organization (UNESCO) report that contains data on water consumption versus availability: it was predicted that two to seven billion people will be faced with water scarcity by the middle of this century. In addition, approximately 800 million people lack quality water and above two billion people lack essential facilities for water usage and production specifically in Africa and Asia continent respectively (United Nation Children's Fund (UNICEF) and World Health Organization. The shortage of water resources calls for efficient techniques for wastewater reclamation. Conventional water treatment is based on the type of contamination which can be sequestered by steps such as coagulation-flocculation, filtration and disinfection. Meanwhile, pollution has aggravated the water shortage problems, different contaminants such as heavy metals and micro pollutants enter water resources from anthropogenic activities. Some of these pollutants are not removed from water totally using non-conventional and conventional water treatment methods. The main challenge now is to develop an adsorbent that will simultaneously remove contaminants present in wastewater. Nanomaterials have been identified as a perfect adsorbent for this purpose due to their physicochemical properties. They also have high surface-active site to volume ratio and controlled pore size distribution, an outstanding and unique properties compared to other adsorbents. This presentation focus on the development of nanocomposites filtration techniques for treatment of industrial wastewater for agricultural purpose.

The Ideal Nanotechnology Solutions for Industrial Scale Water and Wastewater Treatment in Africa

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The use of nanoscale materials and technologies in water and wastewater treatment as a viable and sustainable option will be presented. Focus will be nanotech-enhanced solutions for application in wastewater treatment, including metals recovery, and seawater desalination with emphasis on cost, environment compatibility, energy-efficiency, and ease of production. Africa has an abundance of natural resources and solar energy that can be harnessed by taking advantage of the unique properties associated with nanotechnology-based solutions. Some examples of such solutions (e.g. bionanoflocullants, solar and membrane distillation) will be presented with discussions of the opportunities and challenges that exist.

Keywords: Nanotechnology, biomaterials, water and wastewater treatment, energy-efficiency, environment compatibility

Waste To Value: How can we Effectively Convert Waste into Useful Materials?

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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 overwhelm its recyclability [2], and as such these 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 demonstrate 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.

Keywords: Waste, Pollution

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Synthesis and Characterization of Zeolite a from Ahoko Nigerian Kaolin without Calcination

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Zeolite A $Na_{12}(AlO2)_{12}(SiO2)_{12}$ $.27H_2O$ are micro porous aluminosilicates generally used as a commercial absorbent in nuclear fuel processing and other application. Zeolite A has an alpha cage which comprises of 8 cuboctahedra connected by 12 cuboids which result in a high-quality ion exchange capacities without any known impact in the environment. The work was aimed at Synthesis of Zeolite A from Ahoko Nigeria Kaolin without Calcination. This process was carried out through two different routes, the hydrothermal synthesis route without calcination and the alkali fusion route without calcination. The hydrothermal synthesis route comprises of four different process which are; kaolin pretreatment, leaching process; neutralization and crystallization. This process was carried out by varying concentration of sodium hydroxide at a temperature of 190°C. The second route comprises of four different process which are; Alkali fusion, Gel formation, Gel ageing and crystallization. This process was carried out by varying the ageing time. From the result calculated it shows that molarity of the alkali solution plays an important role in crystallinity of final product. Where percentage crystallinity of 1M NaOH was calculated to be 50.03%, 2M NaOH was calculated to be 63.39%, 3M was calculated to be 76.14% and 4M was calculated to be 94.57% which was calculated from the XRD characteristics peak for different synthesized Zeolite A. From the result calculated it clearly shows that the 4M NaOH at 190°C has a higher crystallinity value with no impurity. Result obtained was compared with the standard value of Zeolite A which shows that result obtained from XRD analysis yields a positive result. The product of the new route possesses a more uniform particle size and morphologies, higher brightness and enhanced cation exchange capacity than the conventional technique for the synthesis of zeolite A through calcination.

Keywords: Zeolites, Kaolin, Synthesis, calcination, Crystallization,

Electrochemical Sensor for Dioctyl Phthalate Based on Molecularly Imprinted Polymer Modified Screen-Printed Electrodes

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Phthalate esters (PEs) are classified as endocrine disruptors and their presence in the environmentis a worrying fact. Their detection in the environment is based non-selective adsorbents for sample preparation and heavy GC-MS investment, thus the need for affordable and selective techniques. The present study developed an electrochemical sensor method based on electropolymerized molecularly imprinted polymers (E-MIPs) for the determination of dioctyl phthalate (DOP). E-MIPs were electropolymerized on commercially available screen-printed electrodes (SPEs) using the cyclic voltammetry (CV) technique, with water-soluble 4- aminophenol as functional monomer and DOP as the template. E-MIPs for DOP showed affinityfor the template, with 80% binding efficiency and an imprinting factor of 3. The E-MIPs were able to detect 250 µg of DOP (equivalent to 12.8 µM) in a time-dependent adsorption manner in5 min. The E-MIPs method reported a limit of detection (LOD) of 9 µM making it suitable for the measurement of DOP in freshwater when the sample is pre-concentrated.

Keywords: Molecularly imprinted polymers, MIPs, Electrochemical sensor, Dioctyl phthalate (DOP), Environmental pollution, Endocrine disruptors.

Integrated Anaerobic and Ozonolysis Treatment of Sludge for Improved Biodegradability and Struvite Recovery

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Municipal wastewater remediation through the activated sludge treatment (AST) system is widely applied. The AST process produces excess biomass separated in sedimentation tanks as waste-activated sludge (WAS). The WAS consists majorly of biomassfrom cell growth and decay, nutrients, and odorous and volatile organic compounds, thus posing the risk of secondary environmental pollution. Anaerobic digestion (AD), the preferredtreatment technique for WAS management, is hindered by the low biodegradability. Therefore, introducing a pre-treatment step such as ozonolysis is necessary for enhancing WAS biodegradability through sludge solubilization. In the current study, integrated ozonolysis pre-treatment and anaerobic digestion of real WAS in fluidized bed reactors was carried out, followed by struvite recovery. Ozonolysis pre-treatment solubilized the extracellular polymeric substances (EPS) in WAS, releasing the biodegradable cellularcontents and increasing the biochemical oxygen demand (BOD5) from 1 520 to 3 520 mg/L.The soluble chemical oxygen demand (COD) increased from 1 700 to 2 300 mg/L with a corresponding increase in dissolved organic carbon (DOC) from 155 to 245 mg/L. Also, the BOD5:COD ratio significantly improved from 0.06 to 0.16, confirming improved biodegradability. Solubilization released the cellular contents into the supernatant, including humic substances, proteins, phosphates, nitrates, and carbohydrates. Sulphates and nitrates increased in the supernatant from 18 to 45 mg/L and 0 to 85 mg/L, respectively, indicating the oxidation of the biomass cell protein. Thermogravimetric (TGA) analysis showed that theweight loss for ozone-treated WAS was 10% while that for the raw WAS was 20%, further indicating that ozonolysis had solubilized the volatile and organic components. In the ensuinganaerobic process, WAS pre-treatment led to an enhanced reduction of the COD and a 230%increase in the cumulative biogas production. Moreover, the nutrients released in the supernatant were easily recovered as struvite (fertilizer) through precipitation with Magnesium Chloride salt.

Keywords: Biodegradation; Ozonolysis; Solubilization; Sludge; Struvite.

Electroactive Low Dimensional Materials for Hydrogen Production from Water Photoelectrolysis

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This presentation focuses on multifunctional 2D and 3D materials and structure/property relationships to control graphene-like and transition metal dichalcogenides nanostructure to be used as three-dimensional hybrid electrodes for hydrogen evolution reaction, sensors and supercapacitors fabrication. We developed a platinum-free electrocatalyst (3D $MoSe_2$ rose-like structure) for the hydrogen evolution reaction (HER) as a first step for large-scale production and application of water splitting devices. Recently, we demonstrated a facile strategy to synthesize decorated molybdenum oxide (MoO_2) nanoparticles on graphene oxide (GO) layers. The hybrid membrane exhibits excellent performance for HER. In the same endeavor, we showed a novel strategy to synthesize vertically aligned porous $MoSe_2$. This designed architecture based on an oriented vertical structure possesses fully exposed active edges and open structures for fast ion/electron transfer, leads to remarkable HER activity with a low onset potential and a 3D binder-free without the need for a transferring step or a conductive additive to build the electrodes. This work opened a new class of nanomaterials in my lab, in which we start the fabrication of photoanodes via in-situ reduction–graphitization approach toward efficient solar hydrogen evolution. For sensing applications, we investigated the direct effect of GO sheets sizes on biosensor performance. For that, we developed a procedure yielding graphene flakes with various amounts of oxygenated defects by using a double liquid phase extraction technique (DLPE) assisted by cholesterol-based polymers and a green method to avoid the use of chemicals and heat to promote the coprecipitation and the reduction of GO and GO based foam (membranes) immobilized aptamer as a highly selective hormone removal. Recent emphasis is on controllable synthesis and development of one-dimensional oriented CdS-based nanoarray photoanodes for efficient solar water splitting / solar hydrogen.

"Green" Synthesis of Cu_2S Nanoparticles from (Z)-1-Methyl-2-(Pyrrolidin-2-Ylidene) Thiourea Ligand for the Preparation of Cu_2s-Chitosan Nanocomposites for the Removal of Cr(Vi) Ion from Wastewater

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The availability of the harmful substances in into our water systems can be a threat to the life of humans and animals, which can lead to serious diseases. The treatment of these toxic substances from water streams can be expensive [1]. Nanomaterials have been used in our days to treat wastewater. Chromium (VI) is regarded as the most harmful and toxic substance due to its high carcinogenic and resistant properties [2]. In this study, the substituted thiourea ligand was prepared, characterized and used to synthesize copper sulfide nanoparticles through homogeneous precipitation. The CuS nanoparticles were then incorporated with chitosan to form Cu_2S–chitosan nanocomposites. The prepared Cu_2S–chitosan nanocomposites were used to remove Cr(VI) ions from wastewater samples. The absorption studies revealed a blue shift in the wavelengths of the band edges when the starch or PVA was introduced into the nanoparticles. The structural studies of the particles were carried out using powder X-ray diffraction (XRD) and transmission electron microscopy (TEM). The emission spectra of Cu_2S nanoparticles in Fig. 1(a) exhibit broad emission maxima which was red-shifted from the absorption band edges. The XRD patterns in Fig. 1(b) presented the cubic $Cu_{1.8}S$ phase for all the synthesized copper sulfide nanoparticles. The adsorption studies proved that the parameters such as pH, dosage and contact time plays an important part during the water treatment. It was noted that when the amount of Chitosan or Cu_2S-chitosan nanocomposites was increased from 0.03 to 0.23 mL, the percentage removal was increasing as shown in Fig. 1(c). The highest percentage removal was achieved at 0.18 mL of the dosage.

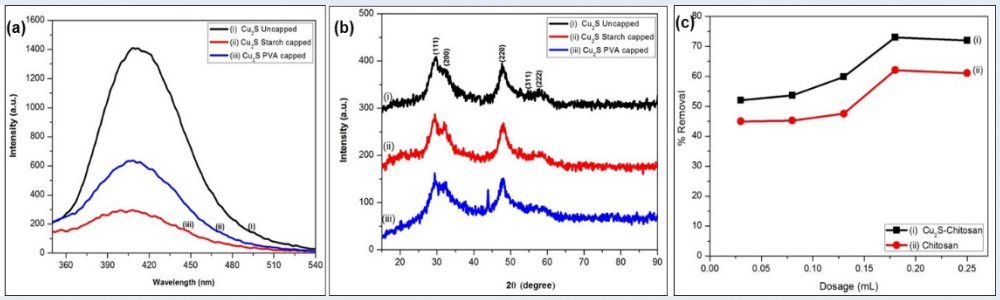


Fig. 1: Emission(a) spectra, X-ray diffraction patterns(b) of Cu_2S nanoparticles and effect of adsorbent dosage(c)

Keywords: Copper sulfide Nanoparticles, Nanocomposites, Chromium (VI) ions & Adsorption

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PRESENTATERS

Extraction and Quantification of Triclosan in Wastewater Samples Using Molecularly Imprinted Membrane Adsorbent

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This paper reports on the successful extraction and quantification of an antibacterial and antifungal agent present in some consumer products (Triclosan: $C_{12}H_7Cl_3O_2$) generally found in wastewater or effluents using molecularly imprinted membrane adsorbent (MIMs) followed by quantification and removal on a high-performance liquid chromatography (HPLC). Triclosan is an antibacterial and antifungal agent present in some consumer products like toothpaste, soaps, detergents, toys, and surgical cleaning treatments. The MIMs was fabricated using polyvinylidene fluoride (PVDF) polymer with selective micro composite particles known as molecularly imprinted polymers (MIPs) via a phase inversion by immersion precipitation technique. This resulted in an improved hydrophilicity and mechanical behaviour of the membranes. Wastewater samples were collected from the Umbogintwini Industrial Complex (UIC), (south coast of Durban, KwaZulu-Natal in South Africa). central UIC effluent treatment plant and pre-treated before analysis. Experimental parameters such as sample size, contact time, stirring speed were optimised. The resultant MIMs had an adsorption efficiency of 97% of TCS with reference to NIMs and bare membrane which had 92%, 88%, respectively. The analytical method utilized in this review had limits of detection (*LoD*) and limits of quantification (*LoQ*) of 0.22, 0.71µgL^{-1} in wastewater effluent, respectively. The percentage recovery for the effluent samples was 68%. The detection of TCS was monitored for 10 consecutive days, where optimum TCS traces detected in the treated wastewater was 55.0µg/L in day 9 of the monitored days while the lowest detected was 6.0µg/L. As the concentrations of analyte found in effluent water samples were not so diverse, this study suggested that MIMs could be the best potential adsorbent for the development and continuous progress in membrane technology and environmental sciences, lending its capability to desalination.

Keywords: Molecularly imprinted membrane, Triclosan, Phase inversion, Wastewater

The Use of Mercury in Gold Mining Activities at Munhena Processing Centre in Manica, Mozambique - an Environmental and Health Effects Assessment

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Gold mining and subsequent processing of mineral using amalgamation techniques are known for their potential contamination to the environment and risk to human health. The Munhena processing centre is a sort of Au city where most families are employed in the Au business. In this site, large number of small-scale miners use mercury in the gold extraction process causing contamination of the environment and risks to human health. Human exposure to Hg was assessed in populations living in this city by means of exhaled air and urine surveys. We also determined Hg concentration in the air, water and sediments using a Hg analyser Lumex RA-915M. The health assessment revealed mercury contamination symptoms, renal damage and high probability of having neurologic disturbances in the studied population. Results of Hg concentrations in environmental samples showed that there was atmospheric deposition of Hg in the study area, accumulation of this metal in sediments and water from the basins used to wash the ore. At present the main concern is that of human health, specifically for those involved in handling Hg and amalgam roasting. Participatory research with small scale miners will have to be initiated to develop practical solutions for the reduction of unacceptable occupational exposure to Hg vapours and Hg losses to the environment.

Keywords: Gold mining, mercury, environmental pollution

Biodegradable Polymer-Based Organoclays for Wastewater Treatment Process as an Alternative to Surfactant-Based Organoclays and Activated Carbon

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Water scarcity has recently become a global challenge as many fresh water sources have been exhausted due to the rapidly growing population and anthropogenic activities. Anthropogenic activities have been identified as a major threat to the environment as they release a mixture of complex pollutants into environment, being polluted water of great concern. To deal with this situation, researchers all around the world are seeking for alternative sources of fresh water. Water reuse has emerged as one of the most promising alternatives for this situation, being wastewater treatment the "trump card" to the success. Adsorption-based technology remains the simplest, well studied and efficient method preferred by most researchers. Activated carbon is the most widely used adsorbents, but the production and regeneration costs combined with the fact that it cannot efficiently remove organic contaminants at higher concentrations have limited its application. As an alternative, organoclays have received enormous attention recently. However, since conventional organoclays are surfactant-based clays, their use raises concerns as most surfactants are harmful for humans, animals, and environment in the event of unprofessional handling or inadequate disposal. It is therefore necessary to develop sustainable adsorbents that can remediate wastewater systems with less or non-negative impacts to humans, animals and without generating other pollution sources. Instead of conventional organo-clays and activated carbon, the present study investigated the potential of using biodegradable polymer-based organo-clays as adsorbents for wastewater treatment.

Keywords: wastewater treatment; organo-clays; biodegradable polymer; organo-modification

Synthesis of Magnetite (Fe_3O_4) Coated Pinecone Crosslinked to Cyclodextrin and its Adsorption Behaviour for 4-Nitrophenol

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Materials for Water and Environment Monitoring Numerous approaches have been studied for the development of cheaper and more effective adsorbents for removal of nitrophenols pollutants from wastewater. In this study, magnetic nanocomposite was synthesized by coating magnetite nanoparticles with sodium hydroxide treated pine-cone by co-precipitation method. Magnetite coated pine nanocomposite was then modified by cross-linking with cyclodextrin using epichlorohydrin. The morphology, composition and magnetic properties of the nanocomposite was characterized using SEM, TEM, FTIR, and VSM analysis. Batch adsorption studies were conducted to investigate the effects of pH, adsorbent mass, contact time and initial concentration on 4-Nitrophenol removal. Pseudo first and pseudo second-order kinetic models were determined to investigate the mechanism of adsorption process. Coefficient of correlation, and variable error, methods were applied in the determination of the best fit of kinetic method. Structural characterization of magnetite coated pine cone (MNPPCP) and magnetite coated pine cone crosslinked to cyclodextrin (MNPPCP-CD) were confirmed by characterization techniques applied. Spherical shaped magnetite nanoparticles with average particle size of 8.23 nm were obtained which increased to 9.77 nm on crosslinking with cyclodextrin. The 4-Nitrophenol uptake onto the magnetite-pine cone nanocomposite was found to be dependent on pH, adsorbent mass and concentration. 4-Nitrophenol efficiency of 9.4 mg/g for MNPPCP and 19.32 mg/g for MNPPCP-CD were obtained at pH 3, when 0.1 g of samples was used at the initial concentration of 100 ppm. Kinetic modelling revealed that adsorption of 4-nitrophenol is controlled by pseudo second-order kinetic model suggesting surface adsorption

Keywords: Co-precipitation; Magnetite; 4-Nitrophenol; pine cone; Cyclodextrin

Highly Efficient Non-Enzymatic Electrochemical Glucose Sensor Based on Carbon Nanotubes Functionalized by Molybdenum Disulfide and Decorated with Nickel Nanoparticles (Gce/Cnt/MoS_2/Ninps)

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Glucose sensing using nanomaterials has recently attracted ever-increasing interest due to the growing demand for sensitive, selective and efficient sensors in pharmaceutical, clinical and industrial settings [1]. In this regard, Carbon nanotubes (CNTs) and molybdenum disulfide (MoS_2) are prospective candidates as effective electrode-specific active materials in electrochemical sensing due to their large surface area and fascinating physical and electrochemical properties [2]. These two nanomaterials, combined with nickel nanoparticles (NiNPs), which are highly attractive for glucose electro-oxidation with high catalytic activity [3], allowed us to develop a new type of CV/CNT/MoS_2/NiNPs-based electrochemical sensor, which are very useful for electrochemical and non-enzymatic glucose sensing. After electrochemical (cyclic voltammetry and electrochemical impedance spectroscopy) and spectroscopic (X-ray Diffraction, Infrared, and Scanning Electron Microscopy) characterizations, the electro-catalytic behavior of the sensor thus designed for glucose oxidation was analyzed by cyclic voltammetry and by amperometric measurements in alkaline medium. The results obtained showed that the sensor has an excellent sensitivity of 1212.1 µA/mM/cm^2 with a wide linearity range (0.05-0.65 mM), a low detection limit of 0.197 µM and a short response time (3 seconds) for glucose detection. Moreover, we have been able to demonstrate through various tests that this sensor has an acceptable level of stability, sufficient reproducibility and repeatability, and ultimately, a substantial preference towards glucose. This explains why the sensor was successful in determining the amount of glucose in samples of the popular 3X drinks in Senegal. The proposed electrode is a good candidate for the creation of non-enzymatic glucose sensors, based on the very satisfactory results obtained.

Keywords: Glucose, non-enzymatic sensor, amperometric detection, and nanomaterials.

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Polymer-Functionalized Graphene Oxide Nanosheets for the Adsorption of Heavy Metal Ions in Water

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Contamination of water sources by heavy metals emanating from acid mine drainage (AMD) can have negative consequence for human and aquatic health. Herein, we report the synthesis, characterization and application of polymer-grafted graphene oxide (GO) nanosheets for the adsorption of mercury and uranium ions from AMD contaminated waters. Surface initiated polymerization (SIP) was used to grow polymer brushes on the surface of GO nanosheets prepared using the improved Hummers method. An initiator, a-bromoisobutyryl bromide, was attached to the GO followed by the polymerization of poly (glutamic acid) (PGLU) using atom transfer radical polymerization (ATRP). The resulting materials were characterized using Fourier Transmission Infrared (FTIR), Powder X-ray diffraction (XRD), Transmission electron microscopy (TEM), Scanning electron microscopy (SEM), Nuclear Magnetic Resonance (NMR), surface zeta potential and X-ray photoelectron spectroscopy (XPS). The adsorption of Hg and U ions on the modified and unmodified adsorbents is discussed.

Keywords: Graphene oxide, Surface initiated Polymerization, Mercury, Uranium

Fly Ash derived Zeolite for Gases Separations and other Industrial Applications

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Zeolites are one of the most expensive materials which find broad applicability as catalyst for a variety of industrial processes such as separations of gases, liquid and solid, cationic exchange attributed to their structure with specific surface, well defined pore dimension, and chemical properties. The coal fly ash offers an opportunity to synthesize zeolites in such a way that creates great environmental and economic impacts. This study identified the key synthesis parameters for fly ash-to-zeolite conversion and their effects on the crystallinity and N_2-adsorption performance for applications in air separation process. Precisely, the study presents the fly ash-to-zeolite conversion synthesis zone that yielded the best crystalline faujasite zeolite and synthesis parameters such cationic exchange and Si/Al ratio that improved the N_2-adsorption process. The fly ash used for sourcing the alumina and silica that gave the zeolite formation was obtained from Sasol Coal mining, South Africa. The raw fly ash was subjected to calcination at 850°C prior to fusion with sodium hydroxide at 550°C, which was then dissolved with appropriate volume of deionized water and exposed to an aging step (6 to 24h) before the hydrothermal treatment, filtration and drying. The Energy-dispersive X-ray spectroscopy analysis revealed the coal fly ash composition of 21 wt.% Si, 56 wt.% O_2 and 16.5 wt.% Al_2. The treated fly ash revealed good properties of Si/Al ratio, surface area, thermal stability, increased crystallinity, improved morphology, and N_2-adsorption characteristic of low silica zeolite (faujasite) with good cationic exchange capacity. Thus, the coal fly ash-to-zeolite conversion can gain notice amongst investors due to its potential market value whilst increasing the environmental sustainability associated with generation of wastes which is one goal of sustainable development.

Key words: *Fly ash, Waste management, Zeolite synthesis, Hydrothermal process*

Dephosphatation in Small Scale Wastewater Treatment Plants

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Phosphorus (P) is recognized as the main cause of eutrophication in aquatic environment which causes ecological problems of water resources. 75% of French territory are subject to eutrophication problems [1]. In this context, large wastewater treatment plants with a capacity of over 10000 people equivalent (p.e.) are equipped with phosphorus removal facilities. Small wastewater treatment plants specifically constructed wetlands (less than 2000 p.e) are not due to cost of phosphorus removal treatment. Constructed wetland are inexpensive systems, effective for suspended solids, organic matter, and organic nitrogen removal, but not adapted for phosphorus removal [2-3]. The removal of phosphorus using sorbents seems to be suitable for constructed wetland due to the simple and easy character to implement and its low cost.

In this context, the aim of this work is to study phosphorus removal from wastewater in a fixed-bed column at laboratory scale. The sorbent used has been chosen due to its strong and fast reactivity towards phosphorus. The influence of the sorbent bed height (5, 7.5 and 10 cm) on phosphorus removal has been studied. First results showed a removal efficiency higher than 90% for the three sorbents bed height tested and an initial synthetic solution containing 10 mg P/L. After the sorbent saturation, the results of the adsorption experiments were compared in terms of equilibrium time, quantity of adsorbed phosphorus per g of sorbent. Mathematical models such as Thomas, BDST, and Clark have been applied to the experimental results to identify the mechanism leading the adsorption process of phosphorus (mass transfer, surface complexation). The characterization (morphology, elemental composition, particle size) of the sorbent before and after its use was carried out to understand the mechanisms involved during the adsorption process. Elemental analysis of the solutions after adsorption process showed the presence of Na and Al corresponding to a partial dissolution of the sorbent of 0,15%.

Keywords: phosphorus, wastewater treatment, eutrophication, alumina-based sorbent, fixed bed adsorption

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Plant-Based Bionanocomposites as Modifiers for Tio_2: Towards Greener Photocatalytic Processes

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The developments of photocatalysts technology is generally hindered by the extremely high temperatures used during catalyst preparation which translates to high costs in terms of energy requirements. The high temperatures stem out of the need to form crystalline semiconductors. This is despite the demonstration in several literature that amorphous semiconductors are also capable of driving efficient photocatalytic decontamination processes (Shao *et al.*, 2015; Moshoeu *et al.*, 2020). Amorphous chalcogenides can be prepared at low temperatures and, therefore, are energy efficient as photocatalysts. We hereby investigate the influence of plant-based bionanocomposites as modifiers for titania (TiO_2) composites on the physicochemical properties and the photocatalytic properties.
Amorphous titania-based photocatalytic bionanocomposites were fabricated from plant based adsorptive bionanocomposites. Based on the composition of the bionanocomposites, two types of photocatalytic bionancomposutes were fabricated; one type was based on adsorptive pine-magnetite bionanocomposite (PMC) and the other on acrylic acid grafted pine magnetite composite (GAA). Since the preparation procedure for amorphous TiO_2 eliminates post-synthesis calcination, the photocatalytic bionanocmoposites were inherently doped with carbon and therefore named PMC–a-C,TiO_2 and GAA–a-C,TiO_2. The effect of co-doping the bionanocomposites was explored by addition of N as a dopant to form PMC–a-C, N,TO_2 and GAA–a-C, NTO_2. The characteristics and photocatalytic performance of the bionanocmposites were benchmarked against C, TiO_2 and C, NTiO_2 fabricated under similar conditions as the bionanocomposites. Doping with N and the nature of the bionanocomposites had a significant influence in the morphological and surface properties while the optical properties were shown to be independent of either factor. The synergy of GAA and N-doping had the most pronounced effect on the morphological and surface features as shown by the typical correlation between the decrease in particle size and the increase in surface area. The Photocatalytic performance was evaluated under UV light for the degradation of a dye cocktail consisting of Reactive red 120 (RR 120) and Rhodamine B (RhB), of the same concentration (25 ppm). The dye cocktail was spiked up to pH 8 using NaOH to simulate the pH conditions typical in real textile wastewater. The N doped photocatalysts and bionanocomposites (C, NTiO_2, PMC–a-C, N,TO_2 and GAA–a-C, NTO_2) all followed the zero order kinetics while the other bionanocomposites followed 1st order kinetics with the GAA based bionanocomposites and C,TiO_2 having the highest overall dye removal. The work has hereby demonstrated that acrylic acid capped adsorptive bionanocomposites make suitable modifiers for greener photocatalysts with a performance that is comparable to those of highly crystalline forms of doped TiO_2.

Key words: Plant-based photocatalysts; Green photocatalysis; amorphous titania; doping

Enhanced Photocatalytic Degradation of Indigeneous Dyeing Wastewater of Sodium-Magnesium-Titanium Multiple Doped Zinc Tungstate Nanocomposites Under Natural Sunlight

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The photocatalytic activity of the Na-Mg-Ti doped $ZnWO_4$ nanocomposites were investigated by monitoring the degradation of Indigeneous dyeing wastewater under sunlight irradiation. $ZnWO_4$ nanoparticle was synthesized by a simple sol-gel technique using zinc acetate, sodium tungstate (precursors) and water and ethanol (1:1) as solvents based on Box-Behnken Design. This was followed by doping of the metallic elements of different mole ratios onto $ZnWO_4$ nanoparticles by wet impregnation method. The produced nanomaterials were analyzed by HRSEM, HRTEM, EDX, UV-Visible Spectrometer, FTIR, BET N_2 Adsorption-desorption, XRD and XPS. HRSEM/HRTEM analysis confirmed the formation aggregated spherical shape irrespective of the synthesis conditions while XRD analysis demonstrated the formation of highly crystalline, monoclinic phase of $ZnWO_4$ with a crystallite size of 14.51 nm at the optimum conditions of solution pH (7.5), reaction temperature(30°C) and stirring speed (2000 rpm) and addition of the dopants did not change the phase. The photocatalytic performance of 1%Na1%Mg1Ti, 1%Na1%Mg2%Ti, 1%Na2%Mg1%Ti, 1%Na1%Mg1%Ti doped ZnWO4 showed that ZnWO4 doped with equal mole ratio of Na, Mg and Ti (1:1:1) exhibited 81.5% degradation efficiency of the organic dyes in the wastewater under the following applied conditions: catalyst dose (0.4g), reaction time (60 minutes) and pH (3) respectively. The experimental data best suited to Langmuir isotherm and a reaction kinetic followed Intra-particles diffusion model. The treated decolourised water was also analysed for reduction in the amounts of contaminants such as sulphates, phosphates, carbonates and bicarbonates and it was found that 1%Na1%Mg1%Ti doped with $ZnWO_4$ exhibited excellent catalytic activity than the undoped $ZnWO_4$ counterpart.

Keywords: Photocatalytic technology, Zinc tungstate, Indigenous dyeing wastewater, metal doping

New Ways of Research on the Use of Typha Domingensis and Phragmites Australis: Explore the Use of Molded Pulp to Promote these Plants into Sustainable Food Trays and Characterization of Paper from Typha for Food Packaging Purposes.

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The hot climate of many tropical countries gives rise to several kinds of weeds that are found in waters and wetlands. Invasive plants considered as weeds are a threat to planet earth because they have negative impacts such as: health impacts and difficulties of access to drinking water, increased irrigation costs, economic impact on fishing with a reduction in the surface area of the pond water, livestock watering difficulties, impact on biodiversity. *Typha domingensis* and *Phragmites australis* are endemic and invasive plants in Africa with a high cellulose content. Nearly a decade after the introduction of cellulosic fiber from this plants, several articles ((Pandey et al., 2020) ; (Ishaq et al., 2021); (Ramesh et al., 2020); (Sana et al., 2014); (Moghaddam & Mortazavi, 2016); (Sharma et al., 2021); (Thangavel et al., 2018); (Ly et al., 2019) ; (Hasan et al., 2022)) have been published on the extraction of the fiber, the study of its properties, its applications in composites and the physico-chemical characterization of paper made from this plant. However, no work has been done to further explore the use of these plants to make food trays and papers for food packaging purposes. This article aims to test the molded pulp technology as a new way of valuing these invasive plants in trays for take away meal, but to go deeper into research on the structural, mechanical, barrier, safety and end-of-life characterization of Typha paper coated with Polyolefin and Polylactic acid. The results showed that Typha paper, in addition to being recyclable, has better mechanical properties (14000 MPa) than the conventional Mitsubishi paper (8000 MPa). Also, these plants can be used as fillers for the manufacture of ecological and affordable trays, but with a control of the migration of heavy metals (found in acceptable quantities in the trays) into food.

Keywords: *Typha domingensis*, *Phragmites australis*, Papermaking, trays, food packaging

Design and Fabrication of a Water Filtration System for Effective Particulate and Heavy Metal Removal from Polluted Water Sources in Ghana

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Activities of illegal mining and improper waste disposal have mostly contaminated water bodies in Ghana with, dirt, heavy metals, and other toxins, making it difficult for communities to acquire safe drinking water. The situation in rural areas aggravates due to the lack of decentralized water supply systems. Poor quality drinking water has numerous health complications and is more severe in children under five. In response to the challenge, a water filtration system was designed and modeled with SolidWorks software. A metallic scaffold was modeled and welded with L-shape steels before part assembling. Gray clay was obtained from the Savannah Region in Ghana for molding ceramic filtration units for dirt and particulate removal. Activated carbon was obtained from coconut coir fibers fired at 900 for 30 mins for particulate and heavy metal adsorption. Other agricultural wastes produced from orange and banana peels were primarily used for heavy metal adsorption. Porous poly-dimethyl-siloxane (PDMS) membrane was obtained via solvent casting and leaching techniques to support the blockage of leaked particles from traveling through the filtration track. Experimental optimizations were done to reduce the turbidity and heavy metal levels in polluted waters. The filtration system proved to be effective in the removal of zinc, cadmium, and copper as well as suspended particulates from contaminated water samples (when compared with WHO recommended limits). Other water quality parameters: pH, conductivity, and turbidity were regularly to ascertain filter duration. The flow rates were determined and compared with the WHO limits. The result and implications were discussed for the optimization of a multipurpose water filtration system for affected communities.

Keywords: Particulate adsorption, heavy metal removal, Porous PDMS membrane, orange peels, and activated carbon.

Novel Heterostructure Catalytic Materials for Removal of Organic Pollutants in Water

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In this three-part presentation, I will discuss work that has been carried out in my group to develop novel catalytic materials for the treatment of organic compounds in water.

In the first part, I will present work on a novel amorphous TiO2-BiOBr-Bentonite multidimensional photocatalyst with very good properties for the degradation of phenol in aqueous solution. The optimized catalyst has a high surface area, low band gap energy and electron-hole pair recombination rate.

In a closely related project, I will present results obtained from the catalytic wet air oxidation of phenol using pillared clay based heterogeneous catalysts. The pillaring method we have developed in the work significantly reduces the pillaring time and water consumption compared to conventional method, indicating advantages of potential scale up of the pillared clay preparation. Excellent catalytic results are obtained for the oxidation of phenol.

Finally, I will talk briefly about work done in preparing modified TiO_2 and ZnO photocatalysts supported on graphitic carbon nitride towards constructing a photocatalytic membrane system for the photodegradation of ketoprofen.

Keywords: Photocatalysis; degradation; catalytic wet air oxidation, nanocomposites, wastewater.

Sulphate Reducing Bacteria (Srb) and Bio-Depollution: An Opportunity for Hann Bay

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Many bacterial species play a beneficial role by participating in both synthesis of recoverable substances and biodegradation of pollutants. Among them we can mention the group of sulphate-reducing bacteria. Sulphate reducing bacteria (SRB) are versatile in their use of various electron acceptors and donors and can also grow under a range of varied environmental conditions. Their growth requires the presence of dissolved sulphate and organic substrates in an anaerobic environment. SRB can also use inorganic carbon (CO_2) such as some species of *Desulfovibrio* genus which have autotrophy capacity. These bacteria can be found in many natural, terrestrial or marine ecosystems. The marine biotope, strongly impacted by human activity, industrialization and urban development, is being degraded by pollution from various origins such as industrial and domestic discharges; and then present health and environmental risks. This phenomenon prevails in Senegal through its bay located in Hann in the area of Dakar. Due to a lack of treatment and operational limitations in the sewerage system (collection constraint, disposal and treatment of liquid waste and rainwater), the bay receives the discharge of large quantities of wastewater, liquid and toxic products from the city center, the suburbs and the heavily polluted industrial area, where more than 80% of industrial structure are concentrated. Once considered one of the most sumptuous bays in the world after Rio, Hann Bay, with its 15 km long has become a real ecological disaster. the current landscape present large dark aquifers that extend in front of wastewater discharges. In view of this situation, communities face multiple challenges, particularly on water quality due to biological and chemical contamination from domestic and or industrial waste (petroleum product, nitrogen and phosphate substance, heavy metal, dyes, agricultural input). Beyond the ecological imbalance, these contaminants have multiple public health implications. To overcome this environmental problem, knowledge of the microbial biodiversity of Hann Bay through the isolation and characterization of bacterial strains of interest, especially those with detoxifying activities under anaerobic conditions, was undertaken. Various samples were taken from this bay and SRB were isolated. The microorganisms were cultured under strict anaerobic, according to Hungate technique. Isolation and purification were carried out by Roll tube method. On these samples, DNA extraction and purification followed by amplification and sequencing of the 16S rRNA gene mainly showed an affiliation to ***Desulfovibrio*** genus with the identification of ***Desulfovibrio alaskensis***, ***Desulfovibrio bastinii***, ***Desulfovibrio thunnarius*** and ***Desulfovibrio desulfuricans*** species. Known for their important ecological role in the carbon and sulfur cycle and, according their metabolic signature, these strains used either individually or in consortium present an excellent opportunity to perform degradation tests and could therefore represent an important vector for bio-remediation.

Keywords: sulphate-reducing bacteria (BSR), marine ecosystem, water treatment, bio-depollution, Hann Bay.

Behavior and Fate of Heavy Metals in Flue Gas from Thermochemical Treatment

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Environmental standards for heavy metal emissions are becoming increasingly restrictive. The flue gas treatment process used in municipal solid waste incineration plants must be improved to control the daily average heavy metals emissions to air with respect to these regulations. Depending on the different operating conditions, it is important to understand the mechanisms of heavy metal transformation during this thermal process. Previous studies have shown that the fate of heavy metals depends on various parameters such as composition of the waste, atmosphere and temperature ([1], -[3]). The aim of this study is to provide a better understanding of the vaporization of heavy metals during gas treatment and to assess the efficiency of heavy metal removal by sorbent. The vaporization behaviors of two heavy metal chlorides ($PbCl_2$, $CdCl_2$) during thermal treatment under air atmosphere, inert atmosphere and a polluted synthetic gas atmosphere are evaluated by thermodynamic equilibrium calculations using FactSage 6.3 software. The results show that increasing the air flow can enhance the vaporization rate of heavy metal. At lower temperature (<450°C) metallic species are mainly in solid form. A complementary kinetics approach is performed using Aspentech software to predict the efficiency of heavy metal removal. Experimental tests are carried out using a laboratory scale tubular furnace which can be heated up to 1000 °C. Various metal chlorides are used as heavy metal sources in gas steam and a sorbent is used to quantify the heavy metals removal. This tubular furnace is connected to two impingers filled with a solution of 5wt% HNO3 to clean up the outlet gas. After adsorption process, the sorbent is characterized to determine the heavy metal concentration adsorbed by elemental to evaluate the removal efficiency. The operating conditions such as temperature, sorbent amount, heavy metal concentration and atmosphere are investigated. Experimental results are compared with simulation results.

Keywords: Gas treatment, heavy metals, kinetics, thermodynamic calculation

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Spotlights on the Structures, Electronic Absorption, and Redox Properties of New Functionalized Monochloro-Triphenylphosphine Ruthenium (Ii) Mono-Dipyridyl Mixed-Ligand Complexes: Potential Materials for Electrochemical Water Splitting System

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It has been recognized in time the technology of hydrogen generation through water splitting at different electrodes by electrolysis using efficient electrocatalysts. Over the last three decades, development of novel materials as electrocatalysts have received great attention as more superior, low-cost, and high performing compounds are being reported. Ruthenium (Ru)-based materials for OER and HER are very promising because of their prominent catalytic activity, pH-universal application, the cheapest price among the precious metal family, and so on. Herein, a systematic molecular design, synthesis, and characterization of new series of five or six-coordinated functionalized monochloro-triphenylphosphine ruthenium complexes having mixed-ligands mono-, dipyridyl complexes are reported. The voltage-current related data obtained from electrochemical oxidation and reduction coupled with the electronic absorption properties form the fulcrum of this report. The cyclic voltammograms (CVs) and square wave voltammograms (SWV) were recorded using the conventional three-electrode system based on a working bare glassy carbon electrode (GCE), Ag|AgCl wire and platinum wire as the pseudo-reference and auxiliary electrodes. The average peak oxidation and peak reduction potentials of the Ru(II/III) redox event range of +1.06 and –0.48 V respectively, while absorption wavelengths and high molar extinction coefficients for the polypyridyl complexes at λ_{max} 265–560 nm ($\varepsilon = 4.170 \times 10^3$ M^{-1} cm^{-1}).

Keywords: $RuCl_2(PPh_3)_3$, mono-, bipyridine acid, uv-vis absorption, electrochemistry, water splitting systems

Strength-Porosity Relationship in Diatomaceous-Based Membranes and the Role of the Aspect Ratio in Filtration Efficiency

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In this ork, the experimental data of strength and porosity from diatomaceous earth membranes are compared with the theoretical models of the minimum solid area also called minimum contact area (MSA) and stress concentration effect (SCE) model. The experimental modulus of rupture was compared with the theoretical models of self-consistency spheroidal inclusion theory and the analytical derived theory. It was observed that the porosity of the membranes affects the behaviour of the mechanical property of the material such that the SCE model fitted more in data obtained from membranes fabricated with a burnout material (charcoal) which had an average porosity of 0.45. Less porous membranes (membranes without a burnout) on the other hand fitted well in the MSA model. The experimental data from the aspect ratio also fitted well with the analytically derived theory.

Key word: Minimum Contact Area, Stress Concentration Effect, Experimental data, Theoretical Models, Strength, Porosity

Best conditions for Optimization of Silica Extraction from Botswana Coal Fly Ash

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This study successfully synthesized high purity mesoporous silica from coal fly ash (a waste produced from the burning of coal in Morupule A Power Station). Two sequential steps were carried out which are the pre-treatment of coal fly ash and the synthesis of silica. In the pre-treatment, coal fly ash was mixed with Na_2CO_3 and then calcined in the muffle furnace. The resultant was cooled to room temperature, washed and dried overnight in an oven. This dried sample was then taken to the next step which is synthesis of silica. Acid refluxing method was used to produce silica from the Na_2CO_3 + CFA thermally activated coal fly ash. Acid concentration and the L/S ratio and their interaction were found to be the most significant variables of the acid reflux synthesis of mesoporous silica. Characterization of the residues carried out were XRF, XRD, FTIR and BET. The silica content from the acid reflux was found to be 99.1% with broad amorphous XRD peak between 20 – 30^O. FTIR spectra mapped very well with the Sigma Aldrich mesoporous silica with BET surface area of 793.5052 m^2/g (pore size 3.9 nm) and 300 – 400 m^2/g (4 nm) of the Sigma Aldrich Silica. Using response surface methodology, the effects of independent variables such as initial MB concentration (50-250 mg L^{-1}), initial pH of solution (3-11), adsorbent dosage (0.1-6.1 g L^{-1}), and contact time (10-90 min) on MB adsorption were optimized. When the pH, MB, and adsorbent dosage were 7, 250 mg L^{-1} and 3.1 g L^{-1}, respectively, the highest MB removal efficiency was 99%. The Langmuir and Freundlich isotherm models were used to test the experimental data, and the obtained data were fully fitted with the Langmuir model (R^2 = 0.9881), indicating monolayer adsorption. The pseudo-second-order model with R^2 of 0.99 was used to predict the adsorption kinetics. As a low-cost and environmentally friendly adsorbent, this synthesized silica can be used widely for water and wastewater treatment.

Keywords: *Coal fly ash, alkali activation, silica, adsorption-isotherms, kinetics*

Organic FETS Using Biopolymer Almond Gum as Gate Dielectric: A Promising Way Towards Green Electronics

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Green electronics is an emerging field of research which aims to manufacture devices in an environmentally friendly and sustainable way. Usually, the involved electronic materials are naturally occurring and non-toxic. Also, they can be processed using simple, low energy deposition processes and fabrication techniques. In this work, we present low voltage organic field-effect transistors (OFETs) using gum arabic (AG) as the gate dielectric. GA is a natural, biodegradable insulator material that can be directly collected from almond trees and used without any further purification. Moreover, GA possesses interesting properties such as water solubility, ease of processing, good insulation, low leakage current, good film quality, and high capacitance making it a promising dielectric for OFET devices. Bottom gate/bottom contact p-channel OFETs have been processed on glass substrates with poly(3,6-di(2-thien-5-yl)-2,5-di(2-octyldodecyl)-pyrrolo[3,4-c] pyrrole-1,4-dione)thieno[3,2-b] thiophene) (DPPTTT) polymethyl methacrylate (PMMA) blend as the active layer and gold as the source and drain electrodes. The transistors operate at low voltage ($V_{GS} \leq 3$ V), with threshold voltages V_{th} as low as -0.8 V, saturated field effect mobilities μ_{sat} above 0.3 $cm^2.V^{-1}.s^{-1}$, subthreshold swings SS around 270 mV/dec and ON/OFF current ratio equal to 10^3. The combined favourable properties of both almond gum and low voltage operated OFET devices have a high potential to pave a way towards using naturally occurring, biodegradable electronic materials in future disposable sensors or throwaway, low-end electronics.

Keywords: Green electronics, almond gum, dielectric, low voltage organic transistors (OFETs)

Porous Organic Polymers as Water Purification Motifs

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Porous organic polymers (POPs) are a class of synthetic material that exhibit properties such as high surface areas, high thermal and chemical stability, and facile synthesis. An assortment of monomers and synthetic pathways results in a wide variety of POPs that can all have different properties and structures. Thus far, POPs have largely been developed for gas adsorption and separation, chemical adsorption, catalysis, sensing, and energy storage. However, the adsorption of aqueous contaminants by POPs continues to be challenging and underexplored area due to their frequently hydrophobic nature.

In this work, a library of POPs have been synthesised using simple Buchwald-Hartwig coupling or condensation reactions. Alternative monomers were identified and incorporated into the reactions resulting in the synthesis of novel POPs. Differences in hydrophobicity were manipulated via monomer feed rations and determined using contact angle measurements. Studies were conducted to evaluate each polymer as an adsorbent of water-based contaminants using a toxic dye as a model. It was shown that through synthetically modifying POPs the performance of the material could be significantly enhanced. The POPs were further functionalised to successfully target toxic dyes, which was not possible with the initial polymers.

The POPs have been successfully incorporated into composites, such as hydrogels or filter tips, to ensure easy use and removal of the adsorbent after the toxic material is absorbed. Use of pH inversions have shown that controlled release of the absorbed materials is achievable leading to recyclability of the networks. Current studies and collaborations are being undertaken to show POPs ability to remove toxic metals, antibiotics, antiretroviral drugs and organic contaminants such as oil or aromatic solvents.

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Potential Application of Multicomponent Photocatalytic – Dispersant System for Oil Spill Remediation

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The potential of semiconductor photocatalysts and environmentally friendly dispersants have been explored greatly in mitigating the harmful effect of crude oil spill. In the present work, the potential application of halloysite nanotubes-Ag-TiO2 (HNT-Ag-TiO_2) composite loaded with binary dispersant mixture made up of Lecithin and Tween 80 (LT80) in remediating oil spillages were examined. The photocatalyst - dispersant composite (HNT-Ag-TiO_2-LT 80) was synthesized via this route; first HNT-Ag-TiO_2 by the photodeposition method using UV irradiation and second encapsulating the Lecithin – Tween 80 dispersant into the lumen of the HNT through vacuum suction. The synthesized composite was characterized by X-ray diffraction, thermogravimetric analysis, Fourier-transform infrared spectroscopy, scanning electron microscopy, and UV-Vis. The HNT-Ag-TiO_2-LT80 composite was active in both the UV and visible light region of the electromagnetic spectrum. The potential of HNT-Ag-TiO2-LT80 as an oil spill remediating material was examined on crude oil and the crude oil fractions aromatics and asphaltenes. The HNT-Ag-TiO2-LT80 reduced drastically the interfacial tension at the oil-water interface resulting in the formation of stable emulsions, smaller oil droplet sizes and high dispersion effectiveness of about 91.5%. A mixture of the oil and HNT-Ag-TiO2-LT80 was subjected to photodegradation under UV light irradiation. The GC-MS and UV-Vis results showed that the photocatalyst - dispersant composite exhibits excellent removal efficiency for crude oil, aromatics and asphaltenes from the oil – sea water mixture depicting that the HNT-Ag-TiO2-LT80 has a great potential as an oil spill remediation material.

Key Words: Emulsification, Photodegradation, dispersant – photocatalyst, crude oil spill, HNT-Ag-TiO_2-LT 80 composite



POSTER **PRESENTERS**

Multi-Application of Fennel (*Foeniculum Vulgaris*) Seed Composites for the Adsorption and Photo-Degradation of Methylene Blue in Water

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This work reports on synthesis of fennel-based composites and their feasibility to remove and photo-degrade methylene blue dye from aqueous solution. Pristine fennel seeds (PFS) was impregnated with iron (III) oxide nanoparticles (Fe_2O_3 NP) and iron (III)-1,2,3,4-tetracarboxylic acid (Fe-TCA) to yield the composites fennel seeds-nanoparticles (FS-NP) and fennel seeds-tetracarboxylic acid (FS-TCA), respectively. Scanning electron microscope (SEM) images revealed that the surface of the adsorbents appeared to have a rough texture with cavities. Fourier transform infrared spectroscopy (FTIR) spectra confirmed the presence of −OH, −C=O, −COC, −COOH and −CO groups that could easily bind to the dye. The physicochemical characteristics such as cation exchange capacity (CEC) and Brunauer, Emmett and Teller (BET) surface area were enhanced after impregnation compared with PFS. The maximum adsorption capacity recorded at pH 10 for PFS was 13.21 mg/g while for FS-NP and FS-TCA was 32.84 and 42.89 mg/g, respectively This was ascribed to chemical interaction such as hydrogen bond, electrostatic attraction and π-π stacking. The isotherm and kinetic data were best described by Freundlich and pseudo-first order models. Thermodynamic parameters (ΔH^o and ΔG^o) showed spontaneity and endothermicity respectively. The positive values of ΔS^o suggests that there was increased level of freedom at solid/liquid interface. PFS showed no activity for photocatalytic degradation properties while PF-NP and PF-TCA recorded 58.97 and 48.62 % efficiencies, respectively. The data revealed that pseudo-second order described the photocatalytic processes of MB better than pseudo-first order kinetics.

Keywords: fennel seeds, adsorption, methylene blue, photocatalyst, degradation, dye

Synthesis of Zinc Chalcogenides Nanoparticles from Substituted Thiourea and Urea Based Zinc Complexes and the Preparation of Nanocomposites for Water Treatment

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Water is an essential resource for human civilization and is the most important substance forall living things in the world. One of the primary humanitarian goals is to have good access toclean water all times; but this remains a problem worldwide. Heavy metals such as lead, iron,mercury and nickel, that are dangerous to human health, are released into the environment through several industrial activities such as painting, smelting, mining, leather tanning and battery engineering. Thiourea and urea are important due to their possible applications in various promising research areas. These substances have been used as drugs and have beenreported to possess an extensive variety of biological activities against bacteria and fungi. Zincsulfide is an important semiconductor with band energy gab. It exhibits better chemical stability than other chalcogenides. Moringa oleifera seeds are known to exhibit coagulation and flocculation properties and these processes have been extensively studied. The ability ofMoringa oleifera to purify water is due to a coagulating/flocculating protein found in its seeds.In this study, zinc urea and zinc thiourea based metal complexes were successfully prepared and characterized.

The zinc complexes were used to synthesis of zinc oxide and zinc sulfide nanoparticles. The effect of temperature was investigated. TEM results of the nanomaterials showed spherical particles. Moringa based nanocomposites were also prepared.

Synthesis of Polypyrrole and Polyaniline Doped with Ionic Liquids, Application of Polymers Films to the Detection and Elimination of Heavy Metals.

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During the last decades, the levels of heavy metals such as copper (Cu^{2+}), lead (Pb^{2+}), cadmium (Cd^{2+}), etc. have continued to increase in food and water. Some of these heavy metals are toxic and pollute the environment. Generally, heavy metals originate from to industrial processes, household waste, combustion of coal, petroleum, etc. Several analysis and separation technics allowing their presence and removal were developed.
The application of polypyrrole (PPY) and polyaniline (PANI) doped by ionic liquids for the detection (of Cu^{2+}) and elimination (of Cu^{2+}, Pb^{2+} and Cd^{2+}) in aqueous solutions was investigated. Firstly, the electrochemical synthesis and characterization of PPy in 1,2- dimethylimidazolium methylsulfate [MMim][MSO_4] was carried out. The PANI was obtained in HCl (1 M) in the presence of two ionic liquids: 1-butyl-3- methylimidazolium tetrafluoroborate (BMimBF4) and 1-hexyl-2,3-dimethylimidazolium chloride (HMMimCl). The PPy film was applied to the detection of Cu^{2+}. The PANI was used in combination with polyvinyl alcohol for the fabrication of cationic exchange membranes. The membranes were characterized by optical microscopy, differential scanning microscopy, thermogravimetry and differential scanning calorimetry.
After synthesis and characterization, the membranes were used for the elimination of Cu^{2+}, Pb^{2+} and Cd^{2+} by electrodialysis technic. The removal percentages of metals vary between 80.63 to 96.04 % (Cu^{2+}), 87.89 to 99.55 % (Pb^{2+}) and 68.33 to 88.03 % (Cd^{2+}).

Keywords: Polyaniline, polypyrrole, onic liquids, Electrodialysis, Membranes, Heavy metal

NonoTechnology for Domestic Water Purification and Reuse.

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In this study, nanoparticles of titanium dioxide (TiO_2) deposited on thin films using electrophoretic deposition (EPD) technique, were applied in photocatalytic degradation of organic pollutants in domestic water. The EPD suspension related parameters and deposition conditions were first optimized for good quality film deposits. The suspension stability and deposition conditions that result in good adherence of TiO_2 particles to the substrate with homogeneous film coatings are ethanol, a TiO_2 solid loading of 4 wt%, a 0.2 wt% iodine concentration in the solvent and a deposition voltage of 20 V in a time of 3.5 minutes. The photocatalytic activity of TiO_2 thin films on domestic waste water decreased exponentially with the ultraviolet light (UV) illumination time and it was also dependent on film thickness, and sintering temperature of the TiO_2 thin films. Highest rate of photocatalytic activity was observed at an optimal film thickness of 95 ± 2 µm sintered at 300 ^{o}C. The implications of these results are discussed for design of inexpensive wastewater domestic purification systems.

Keywords: Nanotechnology, Water purification, Reuse.

Solvothermal synthesis of amorphous TiO_2-BiOBr-Bentonite heterostructures for visible light photocatalytic removal of phenol in water

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A simplistic solvothermal process has been used to fabricate novel amorphous TiO_2-BiOBr-Bentonite (A-TiO_2-BiOBr-Bt) multidimensional photocatalysts with A-TiO_2, BiOBr, and Bt mass ratios fixed at 1:3:4, 1:1:2, and 3:1:4 respectively. The obtained photocatalysts were characterized using techniques such as Powder X-Ray Diffraction (PXRD), Scanning electron microscopy (SEM), Transmission Electron Microscopy (TEM), X-Ray Photoelectron Spectroscopy (XPS), Brunauer-Emmett-Teller (BET) analysis, Ultra-Violet Visible (UV-vis) spectroscopy, Photoluminescence spectroscopy (PL), pH drift method, and Thermo-Gravimetric Analysis (TGA). The A-TiO_2-BiOBr-Bt heterostructure with an A-TiO_2:BiOBr:Bt mass ratio of 1:1:2 ($Ti_1Bi_1Bt_2$) displayed the highest BET surface area, sufficiently low bandgap, and electron-hole pair recombination rate. The high number of A-TiO_2-BiOBr p-n heterojunctions, and the Ti-O-Si and Bi-O-Si bonds between A-TiO_2-BiOBr and Bt in $Ti_1Bi_1Bt_2$ lowered its electron-hole recombination rate and enhanced its visible light-harvesting ability. It is for these reasons that $Ti_1Bi_1Bt_2$ exhibited the best photocatalytic activity compared to the other ternary heterostructures with different mass ratios. Within 70 min of visible light irradiation, 150 mg of $Ti_1Bi_1Bt_2$ gave 100% conversion of 100 mL of 20 ppm of phenol with a pseudo-first-order rate constant of 0.0322 min^{-1} at pH 4.0. Scavenging experiments were conducted and it was demonstrated that superoxide radicals ($O_2^{\bullet-}$) and electrons (e−) were the most dominant reactive oxidation species (ROS) responsible for the phenol photodegradation process while holes (h^+) and hydroxyl radicals ($OH^{\bullet}$) also exerted appreciable participation.

Keywords: Photocatalysis; phenol; degradation; TiO_2/clay nanocomposites, wastewater.

Thermodynamic of Photolysis Reactions Study and Micellar-Enhanced of Photochemically-Induced Fluorescence (ME-PIF) Determination of Fenvalerate Insecticide in Surface and Groundwater

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Fenvalerate is a pyrethroid insecticidal acaricide. The insecticide is a particularly hydrophobic pesticide and its solubility in water is very low below 0.1 µg mL^{-1}, which explains the weak photo-induced fluorescence (PIF) in water. In order to increase the sensitivity of the PIF method in aqueous medium, an anionic surfactant (SDS), two cationic surfactants (CTAC and CTAOH) and a nonionic surfactant (Brij-700) were used. Surfactants are capable of dissolving substances that are insoluble in the solvent used. Firstly, all analytical parameters that may affect the sensitivity of the method (excitation and emission wavelength, pH, irradiation time, micellar solvent and temperature) were optimized. Fenvalerate presented one main excitation and emission band in the regions 278-317 nm and 325-358 nm respectively. Optimum pH conditions obtained in the different media are therefore the following; pH12 in water and Brij-700, pH5 in CTAOH, pH6 in CTAC and pH4 in SDS. However, the optimal irradiation time varies between 8 and 12 min in the different solvent. The micellar association constant (Km) of surfactants were determined at different temperature (298 to 318 K). Km values increase with the temperature, which indicates a micellization more favorable at high temperature. In all case, a negative value of ΔG° was obtained, which shows that the association reactions of fenvalerate with the surfactants used are spontaneous. In addition, linearity of the calibration curves evaluated by variance analysis (p-value ≤ 5%), indicates a significant regression. The low detection limits (LOD) values ranging from 0.006 to 160.35 ng mL^{-1} showed a significant enhanced the sensitivity of the PIF method. Satisfactory means recovery rates varying between 84.0 and 113.2% were obtained in the natural waters by the SPE procedure. Analytical interest of the improved PIF method is that it is better suited to the analysis of insecticide residues in environmental matrices.

Keywords: Fenvalerate; Insecticide; Enhanced photochemically-induced fluorescence; Surfactants; Natural water analysis.

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KEYNOTE SPEAKERS



Paul S. Weiss *graduated from MIT with S.B. and S.M. degrees in chemistry in 1980 and from the University of California at Berkeley with a Ph.D. in chemistry in 1986. He is a nanoscientist and holds a UC Presidential Chair and a distinguished professor of chemistry & biochemistry, bioengineering, and materials science & engineering at UCLA, where he was previously director of the California NanoSystems Institute. He also currently holds visiting appointments at Harvard's Wyss Institute and several universities in Australia, China, and South Korea. He studies the ultimate limits of miniaturization, developing and applying new tools and methods for atomic-resolution and spectroscopic imaging and patterning of chemical functionality. He and his group apply these advances in other areas including neuroscience, microbiome studies, and high-throughput gene editing. He led, coauthored, and published the technology roadmaps for the BRAIN Initiative and the U.S. Microbiome Initiative. He has won a number of awards in science, engineering, teaching, publishing, and communications. He is a fellow of the American Academy of Arts and Sciences, the American Association for the Advancement of Science, the American Chemical Society, the American Institute for Medical and Biological Engineering, the American Physical Society, the American Vacuum Society, the Canadian Academy of Engineering, the Materials Research Society, and an honorary fellow of the Chinese Chemical Society. He is the founding and current editor-in-chief of ACS Nano.*

Nanotechnology Approaches to Biology and Medicine

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Biology functions at the nanoscale. Thus, there are special opportunities not only to make biological measurements using nanotechnology, but also to interact directly in order to influence biological outcomes. I describe how we fabricate and use nanostructures to advance high-throughput gene editing for cellular therapies targeting genetic diseases, such as Sickle Cell Disease, and cancer immunotherapy. We also use microfluidics and functionalized nanostructured features in the selective capture, probing, and release of single circulating tumor cells in liquid biopsies in order to diagnose cancers and to assess the efficacy of treatments. We exploit supramolecular assembly, acoustofluidics, specific surface functionalization, and plasmonics to enable these processes. We leverage nanoscale materials properties to enhance cell growth and co-culture in tissue engineering and regenerative medicine.



Prof. Alejandro Sosnik *received his Pharmacy degree from the Faculty of Pharmacy and Biochemistry of the University of Buenos Aires in 1994. After two years as junior research scholar of the University of Buenos Aires in the field of organic chemistry (1993-5), he worked as research pharmacist in the Department of Chemistry of the Argentine regulatory agency (equivalent to the US-FDA), a dependency of the Ministry of Health of Argentina (1996). In early 1997, he emigrated to Israel where after obtaining the pharmacist license, he continued his graduate studies, receiving M.Sc. (equivalency, 1998) and Ph.D. degrees in applied chemistry (polymeric biomaterials) from the Casali Institute of Applied Chemistry (The Hebrew University of Jerusalem, Israel, 2003) under the supervision of Prof. Daniel Cohn. In 2003-6, Prof. Sosnik spent a postdoctoral in the laboratory of University Professor Michael Sefton (Institute of Chemical Engineering and Applied Chemistry/Institute of Biomaterials and Biomedical Engineering, University of Toronto, Canada). Between 2006 and 2013, Prof. Sosnik was tenured Assistant Professor of Pharmaceutical Technology at the Faculty of Pharmacy and Biochemistry (University of Buenos Aires) and Investigator of the National Science Research Council of Argentina (CONICET). In this period, he established a research group that worked at the interface of drug crystallization and processing, biomaterials science, nanotechnology and microtechnology, drug delivery and therapeutics of poverty-related diseases. In this context, he supervised three junior staff scientists, five postdocs and four Ph.D. theses at the Faculty of Pharmacy and Biochemistry of the University of Buenos Aires. Prof. Sosnik established the "Ibero-American Network of New Materials for the Design of Advanced Drug Delivery Systems in Diseases of High Socioeconomic Impact" (RIMADEL) of the CYTED Program that gathered eleven research groups and companies of Spain, Portugal, Mexico, Cuba, Colombia, Brazil and Argentina and over 75 scientists and served as its international coordinator in the period 2011-2013. He also served as advisor of several Argentine pharmaceutical companies in scientific, technical and intellectual property issues. Owing to its multidisciplinary background and expertise at the interface of drug research and development and polymeric biomaterials, in 2014, Prof. Sosnik was appointed Associate Professor of the Department of Materials Science and Engineering of Technion-Israel Institute of Technology where he founded the Laboratory of Pharmaceutical Nanomaterials Science and heads the BSc program in Materials Engineering and Biology. He was tenured in 2016 and promoted to the rank of Full Professor in 2020. His current research lines comprise drug self-assembly and crystallization phenomena and processing, polymer and macromolecular chemistry, biomaterials science, colloidal chemistry, hybrid organic-inorganic nanomaterials, mucoadhesive drug delivery systems, nanomedicine, therapy of HIV and tuberculosis, and gastrointestinal diseases and pharmacokinetics. Recently, he developed a novel type of ceramic/polymer nanomaterials for the sono-dynamic therapy of cancer. Prof. Sosnik is the co-author of over 170 peer-reviewed articles, reviews, editorials and book chapters in areas of biomaterials science, nanomaterials, tissue engineering, pharmaceutical research and development and innovation, drug delivery, co-inventor in several patents and patent applications related to biomedical and pharmaceutical innovation and editor of two books.*

Actively Targeted Hybrid TiO_2/polymer Nanomaterials for Sonodynamic Therapy of Cancer

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Sonodynamic therapy (SDT) is a minimally invasive and localized anticancer therapy based on the *in situ* generation of reactive oxygen species (ROS) by combining low-intensity ultrasound (US), oxygen, and a sonosensitizer and it minimizes systemic toxicity. We designed and synthesized a novel type of hybrid amorphous TiO_2/polymer nanomaterials by a sol-gel process that comprises the synthesis and aging of a Ti(IV)-acetone oxo-organo complex, its mixing with different linear and branched poly(ethylene oxide)-poly(propylene oxide) (PEO-PPO) block copolymers and their nanoprecipitation in water [1]. Nanoparticles can be produced with fine size control and we demonstrated that they trigger cancer cell apoptosis *in vitro* [2]. In this presentation, I will introduce the most recent advances on the active targeting of the sono-responsive nanomaterials to solid tumors overexpressing glucose transporters by surface glucosylation and their anti-cancer activity in 2D and 3D tumor models *in vitro*. Finally, their pharmacokinetics and efficacy in subcutaneous xenograft murine models of rhabdomyosarcoma.

Keywords: Sonodynamic therapy of cancer; sono-responsive nanomaterials; ceramic/polymer hybrid nanoparticles; active targeting; glucose transporters

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Dr. Niepa *is an assistant professor of Chemical and Petroleum Engineering at the University of Pittsburgh. He started his academic journey in Côte d'Ivoire after receiving an Associate Degree in Food Science and a research experience at the Pasteur Institute. He then moved to Germany to pursue his education in bioengineering at the* ***University of Dortmund*** *and transferred to Syracuse University. He received his B.Sc. in Bioengineering (2009) and Ph.D. in Chemical Engineering (2014) with honors from* ***Syracuse University****. His doctoral study of the Electrochemical Control of Bacterial Persister Cells focused on developing a technology against drug-resistant and persistent bacteria, which was awarded two US patents. During his Ph.D. study, Dr. Niepa co-founded in 2011 Helios Innovative Technologies Inc. (now Leviant, Inc.), a medical device company that develops automated sterilization systems to fight bacterial cross-contamination. He held a Postdoctoral Fellowship for Academic Diversity at the* ***University of Pennsylvania****, working to develop new methods to study microbial dynamics in artificial microniches and thin films. Since 2017, he leads the microBiointerface Lab (at Pitt) in multidisciplinary approaches to solve problems associated with microorganisms relevant to the environment, healthcare, and food industry. He is the recipient of the* ***2022 NIH Director's New Innovator****, the* ***2022 NSF CAREER****, and the* ***2019 NSF S-STEM Awards*** *to promote diversity and excellence in engineering research and education.*

Nanocultures: High-Throughput Platform for Assessing Microbial Community Dynamics in Sessile Drops

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The need for assessment tools for microbial dynamics has necessitated the miniaturization of cell-culturing techniques and the design of microsystems that facilitate the interrogation of microorganisms in well-defined environments. The nanocultures are such an assessment tool: nanoliter-sized microcapsules generated using a flow-focusing microfluidic device to sequester and cultivate microbes in a high-throughput manner. Each nanoculture begins as a nanoliter droplet of cell suspension encapsulated by a polydimethylsiloxane (PDMS) membrane. By manipulating the chemistry of their polymeric shell, the nanocultures can achieve functionalities, such as selective permeability facilitating the transport of metabolites and other small molecules essential to cell growth and community dynamics. The nanocultures allow the diffusion of antibiotics, signaling molecules, and functional fluorescent probes to interrogate cell physiology and facilitate microbial interactions across the confining vessel. Alternatively, multiple species of microbes can be co-cultured within the nanocultures. Because of the chemical exchange occurring within and across the shell, the nanocultures can help investigate microbial pathophysiology. Here, we demonstrate this platform by exploring broad ranges of direct and indirect microbial dynamics. This versatile new tool has broad potential for addressing biological questions associated with drug resistance, chronic infections, antibiotic discovery, and microbiome dynamics relevant to complex microbial communities.

Keywords: bacteria, nanoculture, microbiome, synthetic community, microbial dynamics.



INVITED SPEAKERS

Modifying Materials Using Rod Shaped Fillers: Structured and Functionalized Cellulose Nanomaterial Nanocomposites

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Cellulose nanocrystals (CNCs) are high-aspect ratio, mechanically stiff fibers which can serve as both a bio-renewable reinforcing agent in nanocomposites, as well as a handle for adding stimuli responsiveness. CNCs can be extracted from a wide range of natural cellulosic materials, with characteristics such as crystal structure, crystallinity and aspect ratio fluctuate widely between sources. Moieties attached to the surface of cellulose nanocrystals show that both irreversible and reversible changes can be induced by application of an external stimuli. Our present research focused on the design and fabrication of structured cellulose nanocrystals foams and nanocomposites for implantation. These specifically designed materials are mechanically tunable, matching the intended implantation site.

Keywords: Metal-matrix-composites, polymer-composites, cellulose nanomaterials, reinforcement, stimuli responsive

From Gene to Diagnostics - in Low Resource Settings

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Biosensor-diagnostics used in low- and middle-income countries (LMICs) are high cost when taken in the local context. The required biological reagents for these diagnostics are usually 50-85% of their total materials cost. We will report on biological materials for diagnostics that can be manufactured locally, with basic infrastructure. A **'gene to diagnostic'** approach, with multifunctional fusion enzymes, produces a rational design for point-of-care diagnostics. This is demonstrated for loop-mediated isothermal amplification (LAMP) in nucleic acid tests with BST large fragment (BST_{LF}) DNA polymerase as a fusion protein, isolated on silica via a fused R5 silica-affinity peptide and used in nucleic acid diagnostics. Data from a clinical study of malaria are presented, showing the limit of detection depended on *Plasmodium* species and primer set. For example, 1000 copies of *P. knowlesi* 18s rRNA could be detected with the P.KNO-LAU primer set, but even 10 copies of *P. ovale* 18s rRNA could be detected with the P.OVA-HAN primer set. The results are compared with qPCR and show the local test can meet the WHO recommended guidelines.
The principles are further applied to a device for sarcosine determination in urine (as a marker of early-stage prostate cancer) and recent engineering has used single chain antibody (scFv) fusion to produce self-labelling lateral flow devices for low cost green manufacturing. We have the first step towards providing low cost diagnostics in resource poor areas, which could deliver a sustained improvement in healthcare, while also developing the local economy.

Keywords: *in Vitro* Diagnostics, Synthetic Biology, Malaria

Supramolecular Broad-Spectrum Antivirals

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Viral infections are a great threat for modern society, there are thousands of people that die every year because of them (mostly in under-developed countries) and many more have a lower quality of life because of them. Furthermore, it is become apparent that pandemic infection can have enormous consequences on global health as well as on the economy of the entire world. In this talk I will summarize a decade-long effort in my laboratory to develop broad-spectrum antivirals. The approach that will be presented is different from most biological approach as it is focused on an extracellular mechanism that affect the structural integrity of the virus rendering them non infective irreversibly. I will discuss the development of the compounds that we are investigating and their putative mechanism. In vitro, ex vivo, and in vivo example of the efficacy of such compounds will be discussed.

Using Proteins in Designing Advanced Functional Biomaterials

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Proteins are naturally biocompatible, biologically/ chemically diverse, and exhibit (un)folding nanomechanics under stress/release cycles. Using these uniqueproperties to engineer a new class of biomaterials will place protein-based hydrogels as the next-generation materials. Nevertheless, manipulating these materials' mechanical and microstructure properties is still challenging. nControlling the mechanical and microstructure of protein-based hydrogels is limited asit depends on protein concentration, solubility, and stability. For example, using a lowconcentration of bovine serum albumin (BSA) (~ 0.7 mM) generated a weak hydrogel(~ 3 kPa)[1]. On the other hand, we improved the protein-based hydrogel toughness byincreasing the BSA concentration; however, this approach is limited due to maximumprotein solubility. For instance, forming a sample with 4 mM BSA generated a hydrogel with a maximum stiffness of 15 kPa[1,2]. Protein engineering and DNA recombinant technologies have opened new avenues for designing new protein structures[3]. But, some new designs have high minimum gelation concentrations (~ 150 mg/mL), limitinghydrogel synthesis and narrowing their mechanical behavior range[4,5]. The ability to control the stiffness and microstructure of protein-based materials while preserving theprotein's biological functionality will pave the way to expand our toolbox toward engineering naturally functional biomaterials. Recently, various approaches have been proposed to overcome these obstacles. Forexample, we used polymer-protein interactions to increase the stiffness range (up to 6 – folds) for protein-based hydrogels. This method enabled shape programmable hydrogels based on protein (un)folding transitions, which did not previously exist[6]. Additionally, we used the interactions between Zn^{2+} and Cu^{2+} cations and amino acidsto engineer protein-based actuators[7]. During my talk, I will introduce a new method that confers protein-based hydrogels with tunable mechanical behavior (< 17 kPa) and microstructure morphology by controlling the material's crosslinking density while preserving protein folding transitions and concentration. In addition, I will present the recent progress in my teamprojects for using proteins in designing advanced functional biomaterials.

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Biological Fate of Hybrid Nanocarriers for Drug Delivery: Biodistribution, Degradation and Interactions of Nanomaterials in Biological Environments

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The successful clinical translation of nanocarriers strongly depends on their biodistribution, biodegradation and elimination patterns *in vivo*. However, the visualization and quantification of nanomaterials in *in vivo* models is not trivial. A fundamental aspect of the fate of nanocarriers, in relation with their application in drug delivery, is their degradation. The stability of the core and/or the coating in a nanocarrier plays an important role in the delivery of encapsulated drugs. A premature degradation of the core or the loss of the coating may prevent the delivery of drugs to the targeted tissue or result in the rapid clearance of the nanocarrier. In this presentation issues related to the biological fate and stability of nanocarriers(inorganic, polymeric, hybrid) in *in vivo* models will be presented. Biological fate studies willbe conducted by Positron Emission Tomography (PET) and Single Photon Emission Tomography (SPECT). Fate and transformation of the carriers in biological matrixes will be related to their physico chemical properties. By means of advanced radiolabelling strategies and SPECT imaging we will distinguish the fate of nanocarrier coating and core for polylacticco glycolic (PLGA) nanoparticles. The fate of targeting peptides bound to mesoporous silica nanoparticles will be studied comparing the biodistribution patterns of nanoparticles labelled at the core or at the site of the peptide. To trace the degradation of mesoporous silica nanoparticles *in vivo* core shell nanoparticles of hard and mesoporous silica will be prepared and labelled either at the hard core or in the mesoporous shell. By comparing the biodistribution patterns of the identical nanoparticles differing only in the location of the label, the degradation profile of the mesoporous coating will be estimated. Fate and stability of polymeric siRNA nanocarriers will be studied using both radiolabelled siRNAs and polymers.

Keywords: Biological Fate, Nanocarriers, Positron Emission Tomography, Radiolabelling,Degradation

Characterizing Cell-Surface Interactions at the Nanoscale by Back-Focal-Plane Microscopy for Biosensing and Nanoparticle Delivery

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The propensity of cells to interact with nanomaterials has broad applications for diagnostics and therapies. Due to the small spatial scales and dynamic behaviours of live samples, precisely characterizing the nature of these interactions is a major challenge. The lack of detailed data hinders a rational-design approach. Here, we present how a standard fluorescence microscope can be re-engineered in the back focal plane to meet this critical gap. Specifically, we demonstrate two approaches: 3D particle tracking by point-spread-function engineering and nearfield refractometry by supercritical-angle fluorescence microscopy. The advantage of our approach is that it can yield information on the scale of tens of nanometers while being intrinsically compatible with live-cell imaging.

Aptamer-Based Sensing Platform for Therapeutic Drug Monitoring in Oncology

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The detection of small molecules (< 5 kDa) has become very important and has developed a growing interest in different field including health, environment, and food. With respect to healthcare, anticancer drugs are among those small molecules of particular interest.

Therapeutic drug monitoring is the clinical practice of measuring pharmaceutical drug concentrations in patients' biofluids at designated intervals to allow a close and timely control of their dosage. This practice allows the rapid medical intervention in case of toxicity-related issues and/or adjustment of dosage to better fit the therapeutic demand. It becomes particularly important in the treatment of cancer diseases, since anticancer drugs usually show a narrow range of concentration below which they show no efficacy and above which they cause toxicity, generally characterized by severe adverse effects.

We will describe a surface plasmon resonance sensing platform employing an ssDNA aptamer as a selective receptor to detect an anticancer drug, Imatinib, and its main metabolite. The biosensing platform was tested in simple (PBS buffer) and complex (plasma). The results proved the successful development of a quantitative (competitive binding) assay with consistent validation data covering the range of concentrations within the therapeutic window of this drug and a lower detection limit as low as 79.5 ng mL^{-1}.

Conductive Nanobiocomposites for Human Health Monitoring

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With the quick emergence of the internet of things (IoT) in medical applications, conducting polymer nanocomposite (CPC) that combine different smart properties like piezo-resistivity [1], chemo-resistivity [2,3] or thermo-resistivity [3] appear very attractive. The assembly of conductive polymer nanobiocomposite vapour sensors (vQRS) [4–8] into an e-nose present a strong interest for the anticipated diagnosis of serious diseases such as cancers [2] or sores development and healing [9]. Several strategies are presented to meet the expectations of such applications by starting from the synthesis of the transducer's precursors, a special attention will be put on the selection and dispersion of nanofillers into biopolymer matrices, their structuring from the nano to the macroscale by additive manufacturing layer by layer and the characterization of their chemo-resistive properties. Different ways to tailor the chemical selectivities of vQRS by the hierarchical assembly of conductive polymer nanobiocomposite of different chemical natures will be presented. In particular, the potential of biobased carbon nanorods (CNR) functionalized with poly(lactic acid) PLA and poly(vinyl acetate) PVA were found to detect lung biomarkers at the subppm level. Polysaccharides such as chitosan and amylose can also present an strong interest to functionalize the nanojunctions of the percolated carbon architecture and make sensors have more affinity for polar molecules. Finally, the presentation will focus on data collection and analysis in order to prefigure a diagnosis.

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Chirality and Complexity of Nanostructures: from Catalysis to Vaccines

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Nanoscale chirality is a rapidly emerging field in science and engineering. The early observationof strong circular dichroism for individual nanoparticles (NPs) and their assemblies have developed into a rapidly expanding research area on chiral inorganic nanostructures. They encompass a large family of mirror-asymmetric constructs from metals, semiconductors, ceramics, and nanocarbons with multiple chiral geometries with characteristic scales from Ångströms to microns (**Figure 1**).

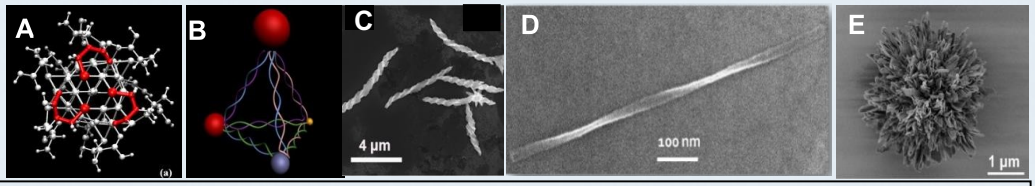


Figure 1. Chiral inorganic nanostructures at multiple scales. (A) Co_3O_4 NPs with twisted crystal lattice ;

Versatility in, scales, dimensions and polarizability of the inorganic materials enables their multiscale engineering to attain a broad range of optical and chemical properties. These capabilities as chiral materials enabled their fast technological translation for biosensing and optoelectronics, which, in turn, opened new venues for scientific inquiry into the unifying rolechirality at the interface of materials science, biology, chemistry, and physics. Some of the latest directions in this field is understanding the fascinating relationships between multiscale chirality and structural/functional complexity of biomimetic nanomaterials forming from the spontaneous hierarchical ordering of inorganic building blocks over multiplescales. Empirical observations of complex nanoassemblies are abundant, but physicochemical mechanisms leading to their geometrical complexity remain puzzling, especially for non- uniformly sized components. These mechanisms are discussed in this talk taking an example ofhierarchically organized particles with twisted spikes and other morphologies from polydisperse Au-Cys nanoplatelets [1]. The complexity of these supraparticles is higher than biological counterparts or other complex particles as enumerated by graph theory (GT).Complexity Index (*CI*) and other GT parameters are applied to a variety of different nanoscalematerials to assess their structural organization. As the result of this analysis, we determined that intricate organization Au-Cys supraparticles emerges from competing chirality-dependentassembly restrictions that render assembly pathways primarily dependent on nanoparticle symmetry rather than size. These findings open a pathway to a large family of colloids with complex architectures and unusual chiroptical and chemical properties. The design principles elaborated for nanoplatelets have been extended to engineering of other complex nanoassemblies. They include polarization-based drug discovery platforms for Alzheimer syndrome,[3] materials for chiral photonics,[5] biomimetic composites for energy and robotics [2,4], CO_2-dispersable catalysis,[6] chiral antiviral vaccines.[7] and pharmaceutical quality control [8]. Yet, the work on the generalization of the engineering principles for chiralbiomimetic nanostructures is incomplete; further directions of these efforts will be discussed.

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Health Simulation in Surgical Orthopaedic Training (SISOT) Using a Natural and Vegetal materiel: The Stem of Bamboo

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The medical scholarship education is based on three keypoints: knowledge, behaviors and skills. The acquisition of the clinical experience and technical skills is no longer simply entrusted to the hospital internship, to the side of a Medical Senior Mentor. During the under and post-graduate medical training, it can also be done in the laboratory of simulation. The learning of the reasoning and clinical approach without forgetting the medical procedures and/or surgical procedures are taught. It forces us to pass by the corpse, the dummy or the animal model for the initiation, the masters and the consolidation of a medical gesture whatever it is: " *Never the first time among the sick* ".

The bone of debit cadaveric became rare or difficult to obtain. The dry bone or synthetic is little accessible because so expensive in the necessary quantities (overabundant numbers) to the modest budgets of our faculties. Also, we are thus condemned to find cheaper support and the physical and mechanical characteristics close to bone's one.

The main research I conduct in the experimental and clinical entity called **Bambou-Sy-Fix (BSF)** and research/ training center called **« Seydi Djamil » Orthopedic Center (SDOC)** address this crucial need. The aims and objective are to work on the substitution to the bone of corpse, the dry bone or synthetic (industrial) as training support to the surgical practice orthopedic and trauma.

Research conducted show that the Bamboo, a source of medical inspiration become an innovative training support-learning and is naturally designated to become our material of choice.

The Bamboo remains thus a natural support, green, biodegradable, sustainable, "Haalal"and accessible with a mecano-similar properties like the human skeletal bone. It remains an irreplaceable tool in the practical training of orthopedic surgeon in our latitudes.

Finally, it represents a good and low-cost medical solution for undeserved regions.

Keywords: Bamboo - Simulation - Osteosynthesis - Osteomyelitis - Orthopaedic training

How Can Nanomedicine Help African Countries to Achieve the Health Sdgs Targets?

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In 2015, UN Member States proposed about 17 Sustainable Development Goals (SDGs) that must all be met by all countries by 2030. The SDG 3 dealt with good health and well-being. The aims of SDG 3 are to end the epidemics of AIDS, tuberculosis, malaria and neglected tropical diseases, and to combat water-borne and other infectious diseases, most of which are major threats to Africa. It also aims to reduce non-communicable diseases by one-third. If African countries want to achieve the SDG 3 targets by 2030, they need to find a technology that will help them to fast-track and overcome health challenges such as nanomedicine. Nanomedicine is the medical application of nanotechnology that promises to offer innovative solutions to unmet medical needs, such as early detection, rapid diagnosis, targeted therapy with fewer side effects, personalized medicine, and effective vaccines.

Keywords: Nanomedicine, health, well-being, epidemic, SDGs

Influence of Characterization and Process Parameters on the Properties of Flax/Epoxy Composites Using Experimental Design System

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This paper presents investigations on the influence of process and test parameters on the mechanical and physical properties of flax/epoxy composites [1] using experimental design method. Specimens fabricated and tested with parameters given by a Doehlert experimental design system [2] have been submitted to quasi-static mechanical loadings, as well as fibre volume fraction and ply thickness measurements. Response surfaces methodology allowed the determination of empirical polynomials corresponding to mechanical responses and to fibre content measurements. The study showed the strong influence of the temperature test parameter on material's mechanical properties and specimens' fracture, followed by compression pressure and number of plies parameters.

Keywords: Flax fibre, Experimental design, Fracture, Mechanical properties, Response surface method.

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Biopolymers and Materials for Health: Applications and Trends.

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Natural biopolymers, polymeric organic molecules produced by living organisms and/or renewable resources, are considered greener, sustainable, and eco-friendly materials. Natural polysaccharides comprising cellulose, chitin/chitosan, starch, gum, alginate, and pectin are sustainable materials owing to their outstanding structural features, abundant availability, and nontoxicity, ease of modification, biocompatibility, and promising potentials. During this conference we aim to overview the most important medical applications of biopolymers and will focus on the chitin/chitosan uses in biomedical field:
-The chemical aspects of Chitin and chitosan derivatives and their potent uses for gene delivery,
- The bioactive-controlled delivery system,
- Wound-healing applications,
- In cardiovascular health,
- As antioxidant, antimicrobial, as Antidiabetic, as Anticancer...

Keywords: Biopolymers, Chitosan, Biomedical, chemical modifications



ORAL
PRESENTATERS

Investigation of the Anti-Obesity Effects of Citrate-Capped Gold Nanoparticles on 3t3-L1 Cells and their Genetic Profiling

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Obesity has been associated with the development of numerous metabolic illnesses, including type 2 diabetes, hypertension, stroke, and certain type of cancers[1]. The current treatment and/or management strategies include lifestyle modification, pharmacotherapy, and surgery[2], however, limitations such as sustaining weight loss[3], toxicity of anti-obesity drugs[4,] and severe complications of surgery[2] remain a huge factor. Recently, the use of nanotechnology in nanomedicine has been regarded as one of the most promising research applications, with nanotechnology offering an exceptional opportunity to improve the treatment of various diseases[5], including obesity. Gold nanoparticles (AuNPs) in specific, have attracted attention and are often preferred for bio-applications due to their remarkable structural and functional properties, including low toxicity, large surface area and the ease of synthesis[6]. In a previous study, we have shown that the exposure of citrate-capped gold nanoparticles (cAuNPs, 14 nm) to human colorectal adenocarcinoma (Caco-2) cells induced non-toxic changes in the expression of certain genes, including genes involved in lipid metabolism[7]. Therefore, in this study, we investigated the cytotoxic effects and anti-obesity activity of synthesized 14nm cAuNPs in 3T3-L1 cells. 3T3-L1 preadipocytes were stimulated with cocktail media to generate obese models. Cell cytotoxicity and cell proliferation assays were performed in 3T3-L1 obese induced cells. Additionally, an anti-lipid accumulation assay was performed in 3T3-L1 obese using different doses of cAuNPs treatments. Treatment conditions that were established to be non-toxic to the 3T3-L1 cells were used to investigate the effect of cAuNPs on the expression of genes involved in cytotoxicity and adipogenesis. We found that cAuNPs were nontoxic to 3T3-L1 cells and treatment of 3T3-L1 cells with cAuNPs reduced triglyceride content at certain concentrations. Additionally, several genes involved in the adipogenesis process were also affected. Therefore, 14nm cAuNPs exert antiadipogenic properties and can safely be used as drug delivery vehicles at specific doses.

Keywords: Nanotechnology, Gold nanoparticles, Nanomedicine, Molecular responses, Anti-lipogenic.

Synthesis, Stability, and Toxicity of Peptide Functionalized Gold Nanoparticles

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Herein, the development of peptide-coated polyethylene glycol gold nanoparticles (Peptide-PEG-AuNPs) as a cellular probe and delivery agent is described. Gold nanoparticles were synthesized and stabilized through chemical conjugation. Thiolate derivatives of PEG were introduced onto the surface of AuNPs. PEGylated-AuNPs contained active binding sites for the immobilization of cancer targeting peptides (p.L, p.C and p.14) using biotin-streptavidin-biotin chemistry. The synthesized AuNPs were characterized using Ultraviolet–visible (UV-Vis) spectroscopy, transmission electron microscopy (TEM), dynamic light scattering (DLS), Fourier transform infrared (FTIR) spectroscopy and electrophoresis mobility assay. Stability of AuNPs and the bioconjugates in physiological solutions (PBS, NaCl and cell culture media) were assessed, the cytotoxic effect of functionalized AuNPs was tested on colon carcinoma (HT-29 and Caco-2 cells), breast carcinoma (MCF-7 cells) and non-carcinoma skin fibroblasts (KMST-6 cells) by employing the 4, 5-dimethylthiazol-2,5-diphenyltetrazolium bromide (MTT) and neutral red uptake (NRU) assay. In present study, citrate-AuNPs were found to be unstable in high ionic solutions, however, aggregation could be prevented with the addition of serum. All peptide-PEG-AuNPs presented no aggregation upon exposure to PBS, NaCl, DMEM and DMEM with 10% FBS. Peptides conjugated to AuNPs were found to have preferential toxicity at higher concentrations as revealed by cell viability assays. Additionally, experiments proved that 14 nm AuNPs could be a source of interference to cell-based assays as depicted by differences between MTT and NRU assay. The final obtained peptide-PEG-AuNP conjugates showed good biocompatibility in the presence of high ionic solutions and biological media (DMEM and DMEM supplemented with 10% FBS) and cellular uptake.

Keywords: Peptide, Gold nanoparticles, Polyethylene glycol, Toxicity, Stability.

Addition of Cu to Ti for Biomedical Dental Alloys

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Biomedical materials are commonly used as structures and implants in humans, to replace lost or diseased biological structures and so improve the quality of life. Every day, more than 14 million people globally suffer from the pain of postoperative infection; 60% of the bacterial infections are related to the use of medical devices. The additions of copper and silver are known to improve the antimicrobial properties of Ti alloys. Copper is one of the more promising alloying elements for clinical applications because of its low toxicity, high cytocompatibility and it is a beta stabilizer. Silver behaves similarly to copper, but it is too expensive to use in industrial applications and is not a good beta stabilizer. There were inconsistencies in the Ti-rich area of the Cu-Ti binary phase diagram, hence the need to ascertain whether Ti_2Cu or Ti_3Cu is formed, and to identify the type of formation.
Four alloys: 20, 33, 40 and 50 Cu (mass%) were produced by arc melting and studied using SEM, XRD and DSC. The reactions were derived from the solidification microstructures of the as-cast samples, and the temperatures of the reactions were determined by DSC. The single peak at 1023°C for the Ti-33Cu (mass%) sample showed that the formation of Ti_2Cu is congruent, and there was an associated $L \leftrightarrow (\beta Ti) + Ti_2Cu$ reaction. The position of the eutectic point was confirmed as being much closer to Ti_2Cu than (βTi), which gave a sparse eutectic that was often difficult to discern clearly, and had sometimes been misinterpreted as peritectic. No Ti_3Cu was found, and this phase is assumed to be metastable, and has also been misinterpreted because of its very similar XRD peaks to Ti_2Cu.

Keywords: Binary system, differential scanning calorimetry (DSC), Ti-Cu, Ti_2Cu

Synthesis and Application of Aptamer Functionalized Quantum Dots for Multiplex Detection of Cancer

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Quantum dots are nanocrystals with unique properties that supersedes other nanomaterials of its class. The quality of size-dependency determines their emission profiles due to the quantum confinement effect which show various colors of light which are ideal alternative to traditional fluorophores for multiplexing studies. The QDs conjugated to biomolecules such as aptamers, antibodies, and protein are applied in various target detection. Various InP/ZnS emission profiles were synthesized and bio-conjugated, their toxicity was tested and bioimaging using protein was conducted. The exciting results will be reported.

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Coal Fly Ash: A Resource for the Development of Materials of Commercial Values

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The continuous dependency on coal to produce electricity results in the generation of coal fly ash which is current constituting several environmental concerns. While coal fly ash disposal has been topical over the past decades, there have been several research interests dedicated to investigating a safe/economic disposal approach either directly or indirectly. This article review some of our research efforts on the utilisation of South African coal fly ash with a view to introduce a seemingly waste material as a resource that can be exploited for the development of materials such as catalyst, absorbent and geo polymeric materials that may find application in chemical and construction industries.

Keywords: catalyst, absorbent, wastewater, coal fly ash, materials, geopolymer

Hygrothermal Characterisation of Typha-Cement Concrete

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The objective of this paper is to investigate the possibility of using typha cement composite material as an insulation material in building. The hygrothermal characteristics and thermal properties of high typha content concrete were investigated.

The results concerning the hygrometric behaviour and hygrothermal characteristics of typha cement concrete are presented. The hygrothermal conductivity of the different formulations was measured by the hot plane method.

Physical results also show that typha is a very porous material. The porosity increases from 23.53 to 39.65% respectively for the fibre percentage from 8.89 to 17.77%.The capillary absorption is very fast in the first minutes for all formulations, it was also found that the more fibrous matrices absorbed more water:

Thermal results as a function of the amount of water in the samples show that Thermal conductivity is difficult to control because of water absorption and desorption. For F250 the thermal conductivity changes from 0.54 to 0.15W/mk over 7 days and for F500 from 0.51 to 0.095W/mk. the thermal effusivity of the samples also decreased progressively for all samples over the 7 days.the typha cement concrete has very interesting hygrothermal properties.

Keywords: (Typha, hygrothermal, porosity, conductivity, effusivity)

Villi Inspired Elastomeric Interlocking Device for Intestinal Retentive Applications

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Achieving prolonged retention of medical devices in the small intestine while mitigating tissue trauma remains a significant clinical challenge. Tissue-piercing microneedles harm intestinal epithelium inducing inflammation while reactive mucoadhesives are susceptible to fouling. Inspired by morphology of the intestinal villi, a mechanical interlocker laminated with high-aspect-ratio elastomeric microposts, that mimic dimensions of the villi, is investigated to develop intestinal retentive platforms. Effectiveness of the interlockers to resist peristalsis is characterized by performing mechanical simulations on Autodesk Fusion 360 and by determining the resistive force applied by villus when it collides with mobile micropost using Euler-Bernoulli beam theory. Interlocking properties are optimized by studying simulation models that investigate the influence of device material properties (50kPa < E_m < 1GPa), micropost pitch, arrangement and tip geometry on the resistive force as the microposts interact with villi under peristaltic shear and contraction. Digital Light Processing 3D printing in tandem with a multi-step replica molding technique is used to fabricate the microposts and artificial villi (E_v= 50kPa). Work of interlocking between fabricated microposts and villi under varying preload and drag velocity is then evaluated through in-vitro lap-shear tests performed on customized equipment to validate simulation results. It is demonstrated that the ability of individual villus to resist movement of a mobile micropost is proportional to the elastic modulus of the micropost and preload. In vitro studies comply with simulation results permitting use of computational approach for future study of elastomeric mechanical interlocking systems. Additionally, interlockers seating 20 round tipped microposts per mm arranged hexagonally can effortlessly consolidate within villi through peristaltic contraction thereby eliminating the need for external stimulation and optimally resist peristaltic shear via mechanical interlocking. These interlockers present a compliant non-penetrative method to develop minimally invasive intestinal retentive platforms for applications in gut diagnostics by indwelling sensors, neuromodulation, and oral drug delivery.

Keywords: Medical Devices, Intestinal Retention, Interlocking, FEA Simulations, Microfabrication

Multifunctional Properties of Bio-Composite: Carbonized Coconut Shell Particles Carbon Fiber Reinforced Polymer Green Composite

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Inorganic fillers have been used to improve the out-of-plane mechanical properties of carbon fiber reinforced polymer (CFRP) composite laminates for decades. Nonetheless, its associated high cost and environmental unfriendliness is a concern. Biomaterials are currently being explored as fillers in polymeric materials due to their low cost, wide availability, and biodegradability. However, the use of coconut shell based biofillers together with carbon fibers in epoxy matrix has not been investigated. This research seeks to improve the out-of-plane mechanical properties of CFRP with low fiber volume fraction using carbonized coconut shell particles (CCSP). Five hybrid epoxy bio-composites with varying concentrations of CCSP were used to impregnate four plies of woven carbon fabric, making up a fiber volume fraction of 29%. The tensile, flexural, impact behavior, electromagnetic interference (EMI) shielding, and thermal behavior of the hybrid bio-composite were investigated. The mechanical properties of the bio-composite laminates were enhanced compared to a reference CFRP without CCSP. The resulting composite exhibits better EMI shielding and thermal stability when compared to a conventional CFRP. The hybrid composite also showed good water absorption resistance as a result of good matrix/fiber adhesion. This work provides a cheaper and greener alternative to inorganic CFRP hybrid composite for potential use in automotive and aerospace industries.

Keywords: Bio-composite, impact test, out-of-plane, electromagnetic interference shielding, and thermal behavior, water absorption

Enhancing Cell-Surface Interaction on Modified Poly-Dimethyl-Siloxane Scaffolds

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Poly-dimethyl-siloxane (PDMS) has been utilized in the fabrication of microfluidic implantable devices for the treatment of medical conditions. This has since been explored in microchannel devices for breast cancer treatment by encapsulating thermosensitive hydrogels. However, the surfaces of the PDMS-based devices have been known to lack contact guidance that promotes cells/tissue-surface interaction. This work is focused on the development of porous-based PDMS scaffolds using the combination of solvent casting and leaching techniques. Three-dimensional (3D) composites porous scaffolds systems were formed using different ratios of Magnetite nanoparticles (MNP) during polymerization for enhanced laser-induced therapy. Results from physicochemical FTIR characterization show a characteristic peak of iron oxide nanoparticles due to Fe-O stretching vibration was recorded at 563 cm^{-1}. Morphological and microstructural characterization using a scanning electron microscope (SEM) revealed micro-macro texturing and large pores on the different systems fabricated. Cell-surface interactions were qualitatively analyzed using immunofluorescent staining of the nucleus and cytoskeleton, while quantitative analysis was done via AlamarBlue assay (a measure of cellular metabolic activity) when 500,000 cells were seeded on scaffolds. The cell-surface interaction outcome, as well as the metabolic processes, revealed that the normal breast cancer cell line (MCF 10A) was supported, while cancer cells (MDA-MB-231) were not favored. Percentage cell viability indicated the porous PDMS scaffold surfaces were more biocompatible when compared to samples incorporated with MNP. The overall outcome of the results would be discussed for the potential application of PDMS scaffolds as implantable drug delivery systems in the treatment of breast cancer.

Keywords: PDMS Scaffolds, IF Staining, morphological characterization, laser induction, and AlamarBlue Assay.

Advanced Multifunctional Nano-Optimised Platform to Retard Actinic Damage and Skin Cancers in People Living with Albinism

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Oculocutaneous albinism (OCA) is a congenital amelanistic pigmentation disorder that affects all known vertebrates and has no known cure. The condition is associated with a partial or complete absence of the pigment melanin. This life shortening condition affecting millions of people is geographically and racially biased towards Sub-Saharan African ethnic groups. Melanin and melanogenesis are the body's primary protection from actinic damage, medically, this damage summarizes all the acute and chronic solar induced adverse dermatological conditions from premature aging, sunburn, solar keratosis to fatal skin cancers. This impairment therefore makes Albinistic persons highly susceptible to all forms of actinic damage as well as susceptibility to bacterial, fungal and viral skin infections.

No treatment has ever been developed specifically to retard actinic damage in albinism. More than 60% of all albinistic persons (living within the tropics and subtropics) with solar keratosis go on the develop cancers including squamous and basal cell carcinomas (SCC and BCC) thereby severely limiting life expectancy. The ineffectiveness of ordinary sunscreens offered to albinistic persons to retard solar induced damage is apparent.

We developed a multifunctional nanotechnology based platform that retards actinic damage in albinistic persons including solar keratosis, which is also antiaging, antifungal and antibacterial. The nano functionalised platform incorporates green synthesis optimised biomaterials conjugated with controlled release drug delivery nano-polymers for optimum transdermal applications on compromised albinistic skin in an aesthetic all day everyday use emulsion. The safety and efficacy of the advanced treatments on albinistic skin types was confirmed using OECD, FDA, COLIPA and CANSA guidelines including clinical trials involving over 2000 persons living with albinism in Zimbabwe.

Key words: Albinism, melanin, actinic damage, solar keratosis, carcinoma

Artificial Enzymes: Synthesis of Nanozymes for Modulating the Immunosuppression of the Tumour Microenvironment (TME)

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Cancer is a leading cause of death worldwide, accounting to the World Health Organization (WHO) accounted to nearly 10 million deaths in 2020.The interaction of tumour cells and the tumour microenvironment (TME) contributes to chemotherapy resistance, relapse, and metastasis. The TME of solid tumours is frequently characterized by low oxygen levels (hypoxia), acidosis (lysosome pH 4-5), and a high concentration of reactive oxygen species. To overcome hypoxia, the tumours require oxygen supply. The nanozymes will be used to provide massive and continuous O_2 production to overcome tumour hypoxia by changing the level of reactive oxygen and nitrogen species (ROS/RNS). Nanozymes are catalytic nanoparticles that mimic natural enzymes. They have superior properties to natural enzymes in terms of stability in harsh environments, have low production costs, and ease of production and modification. Bimetallic (Fe/Mn)/N-Doped carbon quantum dots (CQDs) nanozymes that mimic catalase (CAT), superoxide dismutase (SOD), and glutathione peroxidase (GPx) are synthesized using hydrothermal method in this study. The morphology and size distribution of the nanoparticles were studied using transmission electron microscope (TEM) and dynamic light scattering technique (DLS). The UV spectrophotometer was used to evaluate the CAT/SOD/GPx-like activity of the nanozymes. Cytotoxicity studies against normal and cancer cell lines was also conducted which highlights nanozymes possess anti- and pro-oxidant activity. This research suggests that bimetallic N-doped CQDs can be used as biologically safe nanozymes for anticancer therapeutics, and that they may aid in the development of nanotechnology-based immunotherapeutic.

Electrospinning PVDF – Some of the Challenges

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Properties such as piezoelectricity, lightweight, high thermal stability, abrasion resistance and chemical resistance make polyvinylidene fluoride an excellent candidate for diverse applications.[1] PVDF nanofibers have been extensively investigated to gather insight into the advantages of using these fibers in its applications.[2] Electrospinning provides one of the easy routes to fabricate nanofibers. Our efforts to produce PVDF nanofibers ran into unexpected challenges. Beadless fibers were eventually obtained when DMF/acetone solvent mixture was used to make the polymer solution, along with appropriate salt and surfactants. The presentation will focus on the challenges encountered and how it can be addressed when electrospinning PVDF.

Keywords: PVDF, electrospinning, nanofibers

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POSTER **PRESENTERS**

Influence of Extraction Processes on the Physical and Chemical Properties of Typha Domingensis Technical Fibres.

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Typha domingensis is a monocotyledon plant, belonging to the family typhaceae. It is a fast-growing invasive plant that grows in wetlands [1]. In Senegal, this plant is massively present in the river delta and in other regions of the country. The construction of the Diama anti-salt dam at the end of the 1980s encouraged its proliferation [2].
The objective of the present study is to study the influence of various extraction processes of viable technical fibres from the leaves and stems of typha domingensis plants, on their physical and chemical properties. The extraction methods used are based on retting with sea water, distilled water, and by combing the freshly harvested plants as the mechanical method.
Chemical characterisation by FT-IR and morphological analysis were carried out. The measurements permitted to determine the different chemical groups or bonds, present in the fibres and to their average transverse dimensions. The results showed that the transverse dimensions vary along the length of the fibre, and also as a function of the production process.

Keywords: Plant fibre, retting, mechanical properties, morphology, scattering.

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Nanoindentation and Corrosion Behaviors of 316l AsS and Ti-6Al-4V Alloy in Simulated Body Fluids

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Ti-6Al-4V and 316L austenitic stainless steel (ASS) are the most common biomaterials used in orthopedics and dentistry applications due their good mechanical properties and corrosion resistance. However, they present some limitations in specific environment. In this study the mechanical properties of Ti-6Al-4V and 316L ASS were evaluated using nanoindentation while the electrochemical behaviors were evaluated using potentiodynamic polarization technique in simulated body fluid (Hanks balance salt solution). The corrosion studies of Ti-6Al-4V samples show better corrosion resistance and mechanical properties compared to 316L SS. It was found that δ-ferrite phase is responsible for the corrosion deterioration of 316L ASS. However, heat-treatment of 316L ASS led to phase transformation toward a full occurrence of ϒ-phase as per thermodynamic prediction (Thermocalc), which showed better corrosion resistance but its mechanical proprieties deteriorated from fair to worse.

Keywords: Ti6Al4V alloy, AISI 316 austenitic stainless steel, Nanoindentation, Corrosion

Comparative Study of The Antioxidant Activity of the Mucilage Contained in the Leaves and Bark of the African Baobab (Adansoniadigitata L)

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The baobab tree is native to tropical Africa. In 1592 Prospero Alpino, a Venetian physician and herbalist, gave the baobab the Arabic term "bu-hibab" which means "fruit with many seeds". The baobab (Adansoniadigitata L.) is a tree that grows wild in Senegal [1] and is a good source of mucilage.
The present work focuses on a comparative study of the antioxidant activity of African baobab mucilage contained in leaves and bark, using DPPH as a reagent. Leaf and bark samples were collected from three different sites in the regions of Thiès, Diourbel and Fatick respectively. After drying and grinding the collected samples, we used the extraction method of R. Gaiwe et al [2]. However, for the study of antioxidant activity, we used the method of Kadri et al [3] which is based on the determination of the IC50. The antioxidant activity is all the more important as this value is low compared to that of ascorbic acid (IC50= 4.1298690671 mg/ml). From this study, it appears that the ethanolic and acetone extracts of the leaves showed a better antioxidant activity compared to the ethanolic and acetone extracts of the bark. Indeed, the IC50 value of leaf extracts is relatively low compared to that of ascorbic acid; whereas for bark samples the IC50 values are generally higher than that of ascorbic acid. This difference could be due to the higher presence of polyphenols in the leaves than in the bark.

Keywords: Mucilage; African baobab (AdansoniaDigitata L); extraction, antioxidantactivity, plant organ

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Study of the Photodegradation Kinetics of Fluometuron by UV Absorption Spectrophotometry and Fluorescence

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Fluometuron is an herbicide belonging to the phenylurea family. It can inhibit photosynthesis in small plants [1]. It belongs to a class of pesticides that can undergo degradation that depends considerably on the environmental medium, especially in soils [2]. In order to predict the fate of fluometuron in the aquatic environment and to assess the risk it may pose; we studied its photolysis reaction in aqueous media. This reaction was monitored by UV absorption and fluorescence spectroscopy. A UV irradiation source consisting of a 254 nm mercury lamp was used. The study showed that fluometuron is unstable under the effect of light radiation when irradiated in water. The absorption band and the emission of this product were located at 244 nm and 325 nm respectively. The photodegradation of this product in water has kinetics of order 1 whatever the method followed. In all cases, the half-life times found are relatively low ($t_{1/2} < 1h$). For more information on the photolysis of this herbicide, these two methods were combined with NMR and GC-MS to identify the different photoproducts that may be formed.

Keywords: fluometuron, photodegradation, UV, fluorescence, photoproduits

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SYMPOSIUM-06
NANOSCIENCES & NANOMATERIALS; PHOTONICS MATERIALS



KEYNOTE SPEAKERS



Herbert Winful *is a University Diversity and Social Transformation Professor, the Joseph E. and Anne P. Rowe Professor of Electrical Engineering, Arthur F. Thurnau Professor of Electrical Engineering and Computer Science, and a Professor of Physics at the University of Michigan. He earned a BS degree in electrical engineering from MIT in 1975 and a PhD from the University of Southern California in 1981. After six years as a Principal Member of Technical Staff at GTE Laboratories in Waltham, Massachusetts, he joined the University of Michigan in 1987 as an associate professor of electrical engineering and computer science and was promoted to full professor four years later.*

His many contributions to photonics and quantum electronics include pioneering work on nonlinear optical periodic structures, the nonlinear dynamics of coherently-coupled laser arrays, the physics of quantum tunneling time, polarization instabilities, and distributed-feedback fiber Raman lasers.

Professor Winful is a Life Fellow of the Institute of Electrical and Electronics Engineers, and a Fellow of the Ghana Academy of Arts and Sciences, the American Physical Society, the Optical Society, and the National Society of Black Physicists. His many awards include the State of Michigan Teaching Excellence Award, the Harold R. Johnson Outreach and Diversity Award, and the 2020 IEEE Photonics Society Quantum Electronics Award.

The Birth and Amazing Life of Nonlinear Optics

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The field of nonlinear optics was born at the University of Michigan in 1961 when Franken, Hill, Peters, and Weinreich observed for the first time the generation of optical harmonics. It was indeed a revolutionary act because at the time everyone thought of light as photons and knew that you cannot change the frequency of a photon. That initial observation of frequency doubling of light ushered in the discovery of a plethora of new nonlinear phenomena including optical rectification, third harmonic generation, parametric amplification, self-phase modulation, self-focusing, four-wave mixing, and soliton propagation. Because the optical nonlinearity is fairly weak, the era of nonlinear optics required the invention of the laser, and in particular, the Q-switched laser capable of high peak intensities. Applications of nonlinear optics include the development of new sources of coherent radiation through parametric oscillation and stimulated Raman scattering, the generation of terahertz radiation through optical rectification, the generation of ultra-short pulses through Kerr-lens mode locking, the correction of aberrations through optical phase conjugation, and the generation of entangled photons through parametric down-conversion. Nonlinear optics has made it possible to generate coherent frequency combs that are used in metrology and enable a connection between radio frequencies and optical frequencies. All these phenomena and applications require materials with high nonlinear coefficients that are transparent in the spectral regions of interest. In addition, for even-order nonlinearities the material has to be non-centrosymmetric. Periodically poled lithium niobate (PPLN) and other periodically-poled materials use a technique called quasi-phasematching to achieve highly efficient frequency conversion in practical geometries. High harmonic generation makes it possible to extend nonlinear interactions to the extreme UV and soft x-ray regions. Ultimately, at ultra-high intensities, the vacuum itself becomes nonlinear. Observation of vacuum nonlinearities represents the holy grail of nonlinear optics.

Keywords: Harmonic generation, self-phase modulation, parametric amplification, solitons



***Mmantsae Diale**'s main research interests lie in exploring physical and chemical means to control the electronic and optical properties of materials. She has a keen interest in solar energy conversion with a desire to see a life off the grid with photovoltaics (PV) and artificial photosynthesis (AP) – all green and clean energy sources. Our studies of PV systems involves the work on hybrid organic/inorganic materials for solar cell applications. Furthermore, with AP systems we are working on natural energy conversions 'apparatuses' of plants and algae. This research starts from the basics of physics of materials, structure-property relationships to device fabrication and testing. The significance of understanding the physics and properties of materials will give insight into further developments and actualization of solar devices based on PV and AP. A combination of PV and AP using hybrid system has provided impetus to research in this area, leading to low cost and high efficiency solar cells. MD is an active member of materials research society, having serves as member of academic affairs, symposium organizer and influencing the support for early career researchers. Also, active meber of SAIP, member of council from 2010 -2017 and founder of women in physics in South Africa (WiPiSA).*

Green Synthesis of Eco-Friendly Perovskite Materials for Stable and Highly Efficient Solar Cell.

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The stability and efficiency of HaP solar cells are highly dependent on the quality of the absorber, which is determined by the method and conditions of deposition. For a quick transition from laboratory to industrial scale, safe and scalable deposition methods need to be developed for quality large-area perovskite thin film deposition. Several scalable deposition methods have been explored, including spay-coating, doctor blade coating, screen printing, slot-die coating, gravure printing, ink-jet printing vacuum/vapour assisted deposition. The commonly used solvents in the solution deposition methods are toxic, skin penetrating and carcinogenic. Thus, the development of scalable greener deposition techniques, including scalable solution methods using less hazardous solvents and precise vacuum methods, is much needed for the transition from laboratory to industrial scale. Complete vacuum methods for HaP solar cell manufacturing are eco-friendly, very safe (toxic-solvent free), convenient, and easily scalable. Vacuum deposited HaP thin films have high qualities and stability. To date, most of the developed vacuum techniques control film stoichiometry by checking the rate of deposition. However, the rate of deposition of the HaP precursors fluctuates during evaporation due to the lightweight molecular nature of their vapours. For this reason, techniques involving rate monitoring are not reproducible. The solution to this problem may be to perfect the stoichiometry of the thin film by checking the thicknesses of the precursors instead of the rates. The STVD technique is a physical vapour deposition (PVD) method that involves the optimization of stoichiometry by precisely monitoring the thickness of the precursor thin films using a crystal monitor. This guarantees laboratory-to-laboratory reproducibility of quality HaP thin films.



Mohamed Henini *obtained his first degree at the University of Oran, Algeria. He went to Nottingham University and was awarded the PhD degree in 1984. Mohamed has over 25 years of experience in Molecular Beam Epitaxy (MBE) growth. His particular speciality is the physics and technology of MBE growth for III-V electronic and optoelectronic devices. He has authored and co-authored over 970 papers in international journals and conference proceedings. He has an h-index of 53.*

He is the founder of two international conferences namely, Low Dimensional Structures and Devices (LDSD) and Epitaxial Semiconductors on Patterned Substrates and Novel Index Surfaces (ESPS-NIS). He edited seven books which were published by Elsevier and serves on the Editorial Board of several scientific journals. He is Editor and Associate Editor with Journal of Alloys & Compounds and Materials Today Electronics (Elsevier).

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Emerging Dilute Iii-V Bismides/Nitrides Semiconductors for Photovoltaics Applications

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Following the initial observation by Kondow et al [*Jpn. J. Appl. Phys 35, 1273 (1996)*] that the band gap of GaAs decreases rapidly with the introduction of small quantities of nitrogen, research on the dilute nitrides has attracted a great deal of attention due to interest in its fundamental material physics and potential applications in high efficiency solar cells and quantum well lasers operating at 1.3 μm. However, the optical efficiency of the material decreases with increasing nitrogen content. Potentially, this problem may be improved by co-doping GaAs with bismuth and nitrogen to provide material lattice matched to GaAs. Yoshimoto et al [*Jpn. J. Appl. Phys. 43, L845 (2004)*] have shown that by using low temperature Molecular Beam Epitaxy (MBE) it is possible to incorporate simultaneously both nitrogen and bismuth into GaAs. In addition, in GaNAsBi the combined use of N and Bi could provide a means to control the conduction and valence band *separately*, thus offering interesting possibilities to tailor the band structure to study new quantum phenomena. An important degree of freedom in the epitaxy of III-V semiconductors is the growth of layers on high Miller index surfaces, *i.e.* surfaces oriented differently from the usual (100) orientation. There are several interesting and unusual aspects of non-(100) oriented semiconductor structures related to growth, impurity incorporation, electronic properties (including mobility enhancement of two-dimensional hole gases) and piezoelectric effects. I will report on the MBE growth of $GaBi_xAs_{1-x}$ epilayers deposited on (311) B and (001) GaAs substrates with different As fluxes. The Photoluminescence (PL) and High-Resolution X-ray Diffraction (HRXRD) data obtained from our GaAsBi epilayers indicates that under near-stoichiometric conditions the bismuth incorporation is higher for (311) B growth than for (001) growth. The influence of post-growth annealing on the microstructure and PL will be also reported. A Deep Level Transient Spectroscopy (DLTS) study of defects levels in dilute GaAsN epitaxial layers grown by Molecular Beam Epitaxy (N=0 -1.2%) will be presented. The effects of thermal annealing and hydrogen irradiation on these levels will be discussed.

Keywords: Semiconductors, Photovoltaics, Solar Cells, Defects, Thermal Annealing



Professor Abdoulaye Ndao *received his Master's and Ph.D. degrees in physics from the University of Franche Comte (France). He was subsequently a postdoctoral researcher at UC San Diego and UC Berkeley. His research interests span wide-ranging topics in photonics, material sciences, and physics. He published highly prestigious papers (Sciences, Nature Physics, Nature Communications, Optica, Nanophotonics…) and four patents. In addition, he received ten prestigious awards, including the Kavli: Sculpted Light in the Brain Innovation Grant (2022), Scialog: Advancing Bioimaging Award (2022), Boston University Outstanding Faculty Committee Service Award(2022), Reidy Family Career Development Professorship (2021). "the very best young researcher at Boston University, top ten 2021 Rising Stars of Light, Triton Innovation Challenge grand prize winner for Lidar applications, Prize winner of Institute for the Global Entrepreneur at UC San Diego to name a few.*

Symmetry and Topology in Photonic Nanostructures

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The quest for smaller, lighter, and more efficient optical components usually comes at the price of reduced functionalities. In this talk, I will provide an overview of how topological approach to control light-matter interaction enable novel photonic devices with unique features and enhancedperformance. I will discuss our recent breakthrough in demonstrating the first topological light source that unidirectionally outcouples to a waveguide from magnetic biased photonic crystal cavities of arbitrary shape. I will also discuss the first observation of subwavelength scale Exceptional Points (EP) and their application in biology and healthcare by detecting attomolar concentrations of anti-immunoglobulin G, and the broadest bandwidth achromatic metalens. Suchdevices will be suitable for free space and integrated optics and pave the way towards more complex and versatile systems with applications in high-capacity classical and quantum communications, as well as sensing.



Dr. Moussa N'Gom *is an Assistant Professor in the physics department at Rensselaer Polytechnic Institute (RPI).*

Following an early career in industry as a Sr. research scientist working in the fields of ultrafast lasers, optical communications, and materials processing, he joined the Center for Ultrafast Optical Sciences (CUOS) at the University of Michigan to explore light transmission through highly scattering media through light manipulation or wavefront shaping.

Presently at RPI, in addition to his teaching duties, professor N'Gom conduct fundamental research in quantum optics for quantum communication and the development of a photonics- based quantum computer. He received a NURI grant from the National Geospatial Agency to conduct research on laser filament and its potential ability to 'drill' through clouds for unobstructed Free Space Quantum Optical Communication.

Professor N'Gom holds a BS in Electrical Engineering and Physics from the University of Wisconsin in Milwaukee and a Ph.D. in Physics from the University of Michigan in Ann Arbor.

Producing Multiple Qubits via SpontaneousParametric Down-Conversion

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Solitary optical waves or solitons can propagate indefinitely without an increase in width or a loss of amplitude. Each soliton pulse remains localized within a finite volume, similar to a discrete particle like a proton or neutron. Solitons occur only in nonlinear systems, since nonlinear effects are needed to cancel the natural spreading of the waves as they propagate. Here, we experimentally show that the nonlinear conversion of light carrying orbital angular momentum (OAM) produces coupled optical solitons. Laguerre-Gauss (LG) and Bessel-Gauss (BG) beams are donut shaped optical fields that carry OAM. The second harmonic intensity profile that is generated by these beams are coupled and knotted solitary waves composed of Gaussian spots of various geometries surrounded by concentric rings as shown in Figure 1. The BG input produces two solitons knotted by ellipsoidal rings. The intensity profile generated by LG beams have configurations similar to that of coupled monopoles. The solitons separation is dependent on the fundamental beam topological charge. We show that their spatial profile is invariant against propagation. We observe that their behavior is that of screw dislocations in solitary wave: they collide and rebound at a right angle but retain their identity as they propagate. In this way, we have generated linked frequency doubled optical solitons, that are knotted as they oscillate along the optical axis, when propagating in the laboratory environment. We propose to use these structured optical fields [1] to characterize topologies in materials. Topological defects such as screw dislocations in material systems play a major role in condensed matter physics [2]. Screw dislocations are defects present in periodically ordered structures such as twisted bilayer materials. Such topological material when strongly coupled to these optical solitons can lead to the revelation of a variety of related phenomena whose explanations also rely on topological effects. These light fields together with topological materials will allow for quantum state transfer between bosonic and fermionic systems. This will also allow for the mediation of phase transitions and to determine many distinctive features of materials, from crystal growth to mechanical properties.

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Dr. Souleymane Diallo *currently serves as a program director in the National Science Foundation's Division of Materials Research (Mathematical and Physical Sciences or MPS), supporting the National Facilities and Instrumentation portfolio. Dr Diallo received his PhD in experimental condensed matter from the University of Delaware. His research interests are in the use of neutron and X-ray to interrogate materials and understand their structure-dynamics-property relations. Prior to joining NSF, Dr Diallo was a senior research scientist at Battelle Memorial Institute, working on data analytics/statistical methods for aviation security related projects to support the Transportation Security Agency (TSA). He also worked in industry, most notably as a technical manager for X-ray manufacturer Smiths Detection to support TSA. Dr. Diallo also spent several years as an instrument scientist at the Spallation Neutron Source, Oak Ridge National Laboratory conducting material science focused research and supporting users.*

Neutron Scattering Investigation of the Liquid-Liquid Transition in Confined Water

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Neutron scattering (NS) is a powerful characterization tool used to investigate condensed matter systems and to understand the structure-dynamics-property relation in a wide range of materials applications. The technique is often used to complement X-ray scattering findings, due to its sensitivity to low-Z elements such as hydrogen which would otherwise be invisible. Neutron scattering infrastructures are generally found at large-scale national or international laboratories, such as the NIST-NSF Center for High Resolution Neutron Scattering (or CHRNS). Access to neutron instruments is usually provided at no costs to materials researchers from all scientific background, either via a collaboration mechanism or via a competitive proposal review process.

In this talk, I will introduce the NS technique, describe its current state around the world, and discuss the capabilities and research opportunities that exist at the CHRNS facility for all materials scientists. I will then illustrate our work on the dynamics of water confined in hydrophilic nanoporous silica FSM-12 and FSM-22 (with respectively 16 Å and 39 Å average pore size) in the atto-second timescales. The goals of these measurements are (1) to identify potential changes in the proton momentum distribution $n(p)$ as the temperature is reduced through the putative "fragile" liquid to "strong" liquid crossover temperature T_L, and (2) to determine the lineshape of the corresponding $n(p)$ for comparison with results in other confining media and in bulk water.

Keywords: Neutron Scattering, Confined Water, Phase Transitions, Nanoporous Silica, Nanomaterials



EARLY CAREERS- SPEAKERS



Dr Ibrahima Ngom *is currently a teacher in physics and Chemistry at Senegalese high school. He is also a temporary teacher at the Physic department of Cheikh Anta Diop University of Dakar (UCAD) – Senegal, where he obtained in 2020 his first Ph.D. in the field of the biosynthesis of transitional metal oxide nanoparticles. Dr. Ibrahima Ngom is doing a second Ph.D. in the Physic department of the University of South Africa (UNISA) - South Africa, in the field of nonlinear optical properties of nanocomposites formed between cucurbituril and thulium embedded in porous membranes.*

Ibrahima Ngom obtained in 2001 his Junior High School Teacher's Certificate, option Physic, and Chemistry at Teacher Training School, and then in 2014, he obtained his High School Teacher's Certificate at the Faculty of Sciences and Technologies of Education and Training. Ibrahima Ngom holds his Master's Degree in Physic and Chemistry at UCAD in 2012, and his postgraduate Degree in Physic and Applications, specialization in Materials Science and Engineering in 2015 at the same university.

His research focuses on the biosynthesis of transitional metal oxide nanoparticles (NiO, ZnO, and ZrO_2) using extracts from Moringa oleifera and Adansonia digitata. These nanoparticles can be used for nano-fluids and energy storage systems such as supercapacitors. Dr. Ngom is the author of six publications and he is a reviewer of two international journals.

Study of the Physico-Chemical Properties of Transition Metal Oxide Nanoparticles ZnO, NiO, and ZrO_2 Synthesized from Extracts of *Moringa oleifera*

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This contribution reports on the biosynthesis of transitional metal oxides including nickel oxide (NiO), zinc oxide (ZnO), and zirconium oxide (ZrO_2) using extracts from the flowers, the seeds, and the leaves of *Moringa oleifera*. The nickel nitrate hexahydrate $Ni(NO_3)_2.6H_2O$, the zinc nitrate hexahydrate $Zn(NO_3)_2.6H_2O$, and the zirconium oxynitrate octahydrate $ZrO(NO_3)_2.8H_2O$ are the precursors used for the preparation of NiO, ZnO and ZrO_2 nanoparticles, respectively in the same procedure. All the samples are dried in an electric oven at 100°C and then annealed in the air using an open furnace for 2 h. The NiO and ZnO samples are annealed at 500°C while the ZrO_2 nanoparticles are annealed at 700°C.
The structural, morphological, and optical properties of the materials are investigated via X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, scanning electron microscopy (SEM), transmission electron microscopy (TEM), Ultraviolet-visible - near infrared spectroscopy (UV-Vis-NI) and photoluminescence spectroscopy (PL). All the results show that the nanoparticles synthesized from the leaves of *Moringa oleifera* have small sizes, spherical shapes and are less agglomerated with a more homogeneous size distribution compared to the others. Furthermore, the effect of the annealing temperature on the physical properties of the nanoparticles synthesized from the leaves of *Moringa oleifera* is conducted for the three oxides. The annealing temperatures of the NiO and ZnO samples are 400°C, 500°C, 600°C, and 700°C while those of ZrO_2 are 500°C, 600°C, 700°C, 800°C, and 900 °C. The results show that the crystallite size increases with the annealing temperature and also the band gap evolves towards that of the bulk material.
The nanoparticles thus bio-synthesized could be used in many applications such as wastewater treatment, energy storage devices, or heat transfer fluids.

Keywords: Nanoparticles, biosynthesis, Moringa oleifera, NiO, ZnO, ZrO_2, physical properties



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His research interests cover NLO, nanomaterials for photonics applications and renewable energy. Dr ZONGO authored and co-authored a number of peer-review publications and he is an active member of NanoAfnet and the West African Society of Physics

State of Nanotechnology Research in Sub-Saharan Countries: Opportunities and Challenges

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Nanotechnology is a fast-growing field through advanced research from fundamental to experimental science with a wide range of opportunities limited by challenges. Although nanotechnology demonstrates a broad impact on nearly all industrial sectors of the global economy, namely electronics, energy, water treatment, medicine, telecommunication, aeronautics, defense, automotive, agriculture and environment among others, a very few countries in Africa are making progress in its implementation. Investigation shows a critical lack of strong industry and an ability to translate R&D investments in economic outcome. Furthers barriers are associated not only to the intellectual property rights, but the lack of human and policy capacity. The global scenario suggests the crucial role of cooperation in a multidisciplinary collaboration and partnership between nations, public, private agencies and institutions to boost and move the nanotechnology initiatives toward in Africa.

Keywords: Sub-Saharan countries, nanotechnology initiatives, economy, challenges, opportunities



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Graphene Synthesis by g-Radiolysis

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A simple and economical approach to synthesize Graphene Nanosheets (GNSs) via the exfoliation and intercalation of natural graphite flake material into graphene oxide (GO) following a γ-irradiation process is demonstrated. The GO forms stable colloidal dispersion in polar aprotic solvent and in suspension in N, N-dimethyl formamide (DMF) and in a homogenous phase is reduced by γ-ray induced reduction method which is environmentally friendly and cost effective. The reduction is due to the electrons generated during the radiolysis of DMF. In this study, we report on the physical/chemical characteristics of the γ-ray induced reduced graphene oxide (γ –r GO) suspension adhered on glass substrates.

Keywords: Nanomaterials, Graphene, Radiolysis.



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Dr. Madiba holds a Doctorate degree in Physics with a strong focus in materials science and radiation matter interaction. He is a fellow of the UNESCO-UNISA Africa Chair in Nanoscience and Nanotechnology, Nanotechnology Africa Network and iThemba Laboratory for accelerator Based Sciences. Cementing Africa's fragmented portion of the multidisciplinary Nanoscience and Nanotechnology within the water, energy, and health sector. Dr. Madiba has authored and co-authored over 35 ISI publications as well as participating in various science and engineering conferences. Dr. Madiba is the recipient of the 2015 Swiss government excellence scholarship and an NRF-Y rated researcher within the strategic portfolio of R&D. Furthermore, he serves within the executive board of the African Young Generation in Nuclear, heading the programmes and strategic planning committee.

Materials Under Extreme Conditions: Radiation Effects and Modifications of VO_2 Based Nano-Coatings

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Materials used in space missions can be subjected to various types of radiation including neutrons, gamma, gases, and heavy ions. The damage sustained can be quite complex and simultaneously degrade the characteristic properties of materials. Recently, there has been a growing interest in the development of small satellites with more up-to-date technologies comparable to large conventional satellites in interplanetary space missions. Future development of these small satellites requires the application and use of passive thermochromic layers to achieve good thermal control for longer mission life and cost-effective launches. Vanadium dioxide (VO2) thin films are being considered as an imminent prospect as a passive smart radiator coating (SRCs) for heat regulation in nano and microsatellites. Thermochromic response of VO2 based SRCs is channeled by low emissivity at lower temperatures to preserve the heat, and high emissivity at high temperatures to fritter away the additional unnecessary heat. Since radiation damage induces property modifications in different ways, its radiation tolerance should be investigated. In this review contribution, we discuss a broad overview of radiation interaction with materials. As well as the defects modification characteristics of VO2 thin films subjected to radiation species with energy and projectile doses similar to those accosted in a space environment.

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INVITED SPEAKERS

Multi-Functional Molecular Switches for Energy Efficient Computing and Memory Applications

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Molecular electronic devices are highly complementary to traditional electronic devices and may lead, in principle, to novel functionalities that are very complicated to realize otherwise [1,2]. It has been notoriously difficult, however, to reversibly address molecular switches in solid-state tunnel junctions, but such switches are important to create molecular devices where multiple electronic functions are defined at the molecular length-scales or to develop dynamical systems needed for upcoming technologies, such as, neuromorphic computing.
After a brief introduction to the current status of molecular electronics, i will discuss our recent efforts to develop multi-functional molecular devices [3,4]. Recently, we developed a new type of an electrically driven molecular switch that can toggle between two different functionalities, that of a diode and memory.[5] this dual-functional switch resembles one diode–one resistor (1d–1r) resistive random access memory (rram) but defined within a single molecular layer. This molecular approach is very simple in design, greatly reduces the footprint of devices and the operating voltage (to just <1.0v). By coupling fast electron transport to slow proton addition steps (and associated dynamic covalent bond formation), we are able to create dynamic molecular switches that remember their past [6]. Here, the switching probabilities depend on the operation speed and history of the switches. These switches mimic synaptic plasticity and pavlovian learning. These examples show that electric-field-driven molecular switches pave the way to complex molecular devices where multiple electronic functions are programmed within a single molecular layer.

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Biomass-Based Nanomaterials and Advanced Applications

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The potential of nanotechnology in various sectors of research and application is promising and attracting increasing investment. Unexpected and attractive properties can be observed when decreasing the size of a material down to the nanoscale. Cellulose and other polysaccharides (starch, chitin) are no exception to the rule. In addition, due to their abundance, renewability, high strength and stiffness, non-toxicity, low weight and biodegradability, the highly reactive surface of polysaccharides resulting from the high density of hydroxyl groups is exacerbated at the nanoscale.

Although cellulose is the most available natural polymer on Earth, it is only recently that it has gained importance as a nanostructured material thanks to its hierarchical structure. Cellulosic nanomaterials are generally in the form of cellulose nanofibrils (CNF) or cellulose nanocrystals (CNC). The mechanical modulus of crystalline cellulose is the basis of many potential applications. Moreover, the low thermal expansion coefficient caused by the high crystallinity of cellulose nanomaterials and high transparency without the presence of any existing polymer is highly advantageous for flexible display panels and electronic devices. For papermaking, in addition of improving the tensile strength, burst strength, tear, density, smoothness and also increasing the air permeability, the capacity of retaining the filler and the adsorption of a dye are also improved by the nanoparticles. Besides, the inherent high reactivity of cellulose and the pervasive surface hydroxyl groups associated with the nanoscale dimensions of cellulose nanomaterials open up opportunities to develop new functional nanomaterials.

Keywords: Polysaccharides; Nanoparticles; Nanocomposites.

Upconversion Nanoparticles and their Application in Theranostics

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Light triggered theranostic (*thera*py and diag*nostic*) platforms have gained a considerable attention in recent years. In theranostics, light as an external trigger stands out due to its non-invasiveness, high local precision and temporal resolution. Many such theranostic nanoplatforms employ high-energy (visible or UV) light to initiate the individual therapeutic and diagnostic modalities. However, light at these wavelengths suffers from inherent drawbacks such as having little to no penetration in living tissue, induces autofluorescence from inherent fluorophores or chromophores in tissues and can cause photodamage. The use of NIR light for excitation mitigates such drawbacks associated with high-energy excitation, for example, little to no background autofluorescence from the specimen under investigation as well as no incurred photodamage. Moreover, one of the biggest limitations is of course, that of penetration. As such, NIR light can penetrate tissues much better than high-energy light especially when these wavelengths lie within the three biological windows (BW-I: 700-950, BW-II: 1000-1350, BW-III: 1550-1870 nm) where tissues are optically transparent. At the forefront of NIR excited nanomaterials are rare earth doped nanoparticles, which due to their 4*f* electronic energy states can undergo conventional (Stokes) luminescence and emit in the three NIR biological windows. However, unlike other classes of nanoparticles, they can also undergo a multiphoton excitation process where the NIR excitation light is converted to higher energies resulting in anti-Stokes luminescence spanning the UV-visible-NIR regions (commonly known as upconversion). Due to the versatility of their optical properties, it now becomes possible to generate upconverted high-energy light (UV or blue) *in situ* to trigger other light activated therapeutic modalities (*i.e.* drug release) while using the NIR emission for diagnostics (*i.e.* bioimaging, nanothermometry). Here, we present the synthesis of various NIR excited (and emitting) rare earth doped core/shell (and multishell) nanoparticles and demonstrate how their luminescence properties can be exploited for potential use in theranostics.

Keywords: Rare earths, Upconversion, NIR Luminescence, Nanoparticles, Core/shell

Interfacial Properties in Composite Nano-Systems for Energy Harvesting

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Composite nanostructures can be efficiently applied for Sunlight detection and conversion and, more in general, for energy harvesting and generation of solar fuels. In most of the applied systems, like photodetectors, excitonic solar cells and (photo)-electrochemical cells to produce solar fuels, nanomaterials can play a critical role in boosting photoconversion efficiency by ameliorating the processes of charge photogeneration, exciton dissociation and charge transport. Critical role in such processes is played by the structure and quality of the interface, which needs to be properly assembled to obtain the desired functionality. Several strategies can be pursued to maximize energy harvesting and storage, including broadening of light absorbance to reduce solar light losses, fastening exciton dissociation and charge injection from the photoactive medium to the charge transporting materials, reducing charge recombination during charge transport and collection at the electrodes. In this lecture, a few examples of application of nanocomposites will be discussed, including all-oxide coaxial p-n junction nanowire photodetectors and solar cells, core-shell quantum dot fluorophores for high-efficiency luminescent solar concentrators, composite sulfides for hydrogen generation, and oriented carbon nanotube forest dispersed in polymer matrix as efficient low-temperature thermoelectric composite. Emphasis will be given to the role of interface engineering in improving the efficiency of energy conversion in different systems, spanning from electric power generation from Sunlight, to chemical fuel production, to conversion of heat lost through thermoelectric materials.

Keywords: p-n junction nanowires, quantum dots, interfacial properties, luminescent solar concentrators, solar cells, low temperature thermoelectric composites.

Plasmonic Heterogeneous Photocatalysts Free of Noble Metals

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Heterogeneous photocatalysis is an emerging process allowing the generation of solar fuels from water and CO_2. However, the photocatalytic activity is currently very low. In plasmonic photocatalysis, the semiconducting photocatalyst is decorated with a plasmonic nanoparticle, resulting in a significant increase in photocatalytic activity. However, most plasmonic photocatalysts are based on Au or Ag plasmonic nanoparticles. In this communication, we present our efforts to prepare plasmonic photocatalysts that are free of noble metals. First, we will look at the preparation of plasmonic photocatalysts based on TiN, a wide-band photocatalyst. We will in particular demonstrate that photocorrosion is a significant factor in the interpretation of the results. In particular, a novel Magneli-type titanium oxynitride will be shown to contribute to the high activity of the photocatalyst. Then, we will present results on photocatalysts using Cu plasmonic nanoparticles. For this latter case, photocorrosion is detrimental. Using an innovative polymeric nanoencapsulation technique, we were able to prevent photocorrosion, leading to the formation of Cu-plasmonic photocatalysts with high activity.

Keywords: Photocatalysis, Nanomaterials, Hydrogen, Energy

Role of Heterojunctions in Metal Oxide Heterostructures for Energy and Environmental Applications

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Heterostructures made from metal oxide semiconductors are fundamental for the development of high-performance gas sensors and electrocatalysts, for examples. In this lecture we will introduce hierarchical heterostructures composed of p-, n-type and insulating metal oxide shells.
Precisely controlled films of alternating metal oxides can be uniformly deposited onto the inner and outer walls of the CNTs and onto mesoporous substrates by atomic layer deposition. The morphological, microstructural and electrical characteristics of the heterostructures were thoroughly investigated. Electrical resistance measurements highlighted the large influence of the metal oxides thickness and charge carriers types, suggesting that the conductivity of the electrodes are dominated by the heterojunctions.
The behavior of the heterostructured electrodes in sensors and in electrocatalysis applications was investigated for low concentrations of volatile organic compounds and pollutants, and the oxygen evolution reaction in acidic media, respectively. For examples, the gas sensing response of the heterostructures showed a strong dependence on the thickness of the metal oxide shell layers and the type of heterostructures formed. On the other hand, the electrocatalytic performances are strongly related to the surface catalyst/stabilization layer and the electrical conductivity of the heterostructured electrode. On the basis of the morphological, microstructural and electrical characterization, and electrode performances, the mechanisms which account for the performances of our heterostructured electrodes will be correlated and discussed.

Keywords: Heterostructures, Atomic Layer Deposition, Nanostructured Materials

Eco-friendly Synthesis of zinc oxide nanoparticles using Safran Extract and its photocatalytic and antimicrobial activity

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The use of nanomaterials for environmental remediation represents an ambitious and innovative solution, which guarantees a fast and efficient removal of pollutants from contaminated sites. The present work reports the green synthesis of zinc oxide nanoparticles (ZnO NPs) using an aqueous extract of Saffron leaves. The ZnO nanoparticles were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM). The XRD pattern analysis confirms the presence of a pure wurtzite hexagonal crystal structure of ZnO.

The obtained ZnO NPs were stabilized by the interactions of phenolic compounds present in the saffron plant extract. The ZnO NPs thus prepared to reveal antibacterial activity against three bacteria. The photocatalytic activity of the synthesized ZnO NPs was analyzed for the degradation of methylene blue (MB) dye in sunlight. Almost complete degradation of the dye occurred within 90 minutes. However, this ZnO NP prepared by an environmentally friendly method will be much more useful for dye removal and bacterial decontamination. Consequently, the green synthesized ZnO might be utilized in pollution control, and it will be a breakthrough in the development of more environmentally friendly, sustainable, and innovative nanostructured materials.

Keywords: Safran, Zinc oxide nanoparticles, Green synthesis, Antibacterial activity, Photocatalytic activity, Sustainability.

Architecting the Columnar Morphology of ZnSe Sculptured Thin Films for Polarization-Universal Bandgaps

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Columnar thin films (CTFs) are assemblies of parallel straight columns of nanoscale cross-sectional dimensions grown by physical vapor deposition on appropriate substrates. Sculptured thin films (STFs) are similar, but the columnar shape is architected for specific objectives. With the aim of realizing polarization-universal bandgaps, we architected the columnar morphology to fabricate two types of unidirectionally periodic STFs. The first type is called tightly interlaced matched ambidextrous bilayers (TIMABs), whose unit cell comprises one structural period each of two otherwise identical chiral STFs but of opposite structural handedness. The second type is called equichiral sculptured thin films (ECSTFs), whose unit cell comprises four CTFs that are identical and have the same thickness, except that the substrate had been quickly rotated by 90° about a central normal axis between the depositions of any two consecutive CTFs. Polarization-universal bandgaps with maximum transmittance under 20% were realized as sculptured thin films for TIMABs to modify the circular Bragg phenomenon and ECSTFs that display the Bragg phenomenon for both linear and circular polarizations. The TIMABs and ECSTFs were made by thermally evaporating 99.995% pure zinc selenide at 50 μTorr in a low-pressure chamber. Glass and silicon substrates were oriented on a rotatable substrate holder so that the collimated adatomic vapor of zinc selenide would be directed at an angle $\chi_v = 20^\circ$ with respect to the substrate plane. At least 18 periods were deposited for each film analyzed to ensure a fully developed Bragg regime. The resulting films were between 5 and 7 μm in thickness. Both the symmetric and asymmetric serial bideposition modalities were employed for architecting the nanocolumns. Samples were characterized optically in transmission and reflection as a function of incident angle of light and polarization. The film morphology was examined using scanning electron microscopy on cleaved silicon samples.

Keywords: Bragg phenomenon, structural chirality, physical vapor deposition, polarization state, sculptured thin film

Saving our Environment and Resolving Climatic Issues Through Nanoscience Research

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As the globe's population and energy consumption continue to rise, the world faces tremendous difficulties. Fossil fuels and other raw resources, which are currently the primary sources of energy generation, are depleting at an alarming rate, posing serious environmental and climatic issues. To overcome the problems posed to the environment by using green design and analysis, new research, new concepts, and creative developments in the use of new technologies are required. Innovative research and fresh innovations in the application of new instruments to address the difficulties should be pursued. This is clearly a research-based, thorough, and practical study that focuses on the use of applied concepts to increase productivity and sustainability. As a result, substantial research is provided that reports on new approaches and vital applications in the disciplines of chemical and physical sciences to cope with and protect our corroding environment, as well as providing cleaner and fresher air through nanotechnology. We discuss the synthesis and characterization of nanomaterials for preserving our environment and hence curbing the menace of climatic challenges. We propose development of new materials, perovskite, photo electrochemical and dye sensitized solar cells with a view to developing clean and cheap energy. Over 60% of the light in the visible region transmitted through the electron transporting layer and absorption edge of PbI_2 and $MAPbI_3$ with optical band gap of 2.49 eV and 1.63 eV respectively for a perovskite cell. For perovskite, photoelcetrochemical and dye sensitized cells layers deposited by spin coating, CVD, SILAR and CBD, the efficiencies were calculated to be 0. 046% and 12.89% respectively.



ORAL
PRESENTATERS

Carbon Nanotubes as a Reinforcement Material for Sustainable Construction Composites

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Carbon nanotubes (CNTs) have gained considerable attention in various applications because of their distinct inherent properties arising from their nanoscale sizes. CNTs are characterized by high surface area, aspect ratio, thermal stability, and excellent mechanical strength. In this study, a floating catalyst chemical vapour deposition (FC-CVD) method was adopted to synthesize CNTs. The FC-CVD method is facile as both the carbon source and catalyst are introduced simultaneously into the furnace and can allow continuous CNT production. Multi-walled CNTs (MWCNTs) of high purity and crystallinity were produced with this method and were functionalized by acid reflux to enhance their processability and to ensure homogeneous dispersion in the intended construction composite application. Coal fly ash and waste plastics were used to produce the composites in a unique process. The mechanical properties and the filler-effect of MWCNTs due to their nanosizes facilitated load transfer and reinforced the composites with loadings as low as 0.01 wt%. Thus, producing high-strength composites from waste. The quality of the MWCNT-reinforced composites was assed using a range of techniques and the results will open a new avenue of sustainable and affordable building materials which will be beneficial, especially for developing countries which have a housing and infrastructure deficiency. The manufacturing process also frees the environment from unwanted waste.

Key words: carbon nanotubes, waste plastic, coal fly ash, eco-bricks and sustainability

Enhanced Optoelectronic Properties of TiO_2:Ge Thin Films Annealed in a Nitrogen Ambient

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TiO_2 has attracted significant interest in research due to its interesting properties which have found applications in optoelectronics. For example, it has found application in the photoelectrode in dye sensitized solar cells; devices used for photovoltaics. The properties of TiO2, can be manipulated depending on films composition, deposition method and post deposition treatment to align to the properties of a desired application. In this study, TiO_2 and TiO_2:Ge composite films are deposited using Radio Frequency (RF) sputtering and annealed at 450 ℃ in different ambient (Air, Argon and Nitrogen) in an attempt to compare how the ambient affects the properties of the films. The films were characterized structurally, morphologically, electrically and optically. X-ray diffraction of the films showed both anatase and rutile phases with crystalline structure and crystal sizes of ≈20 nm. Scanning Electron Microscope showed large crystals for the Nitrogen annealed. It was observed that high Germanium content reduced the electrical conduction ($2\ 11\ 10^{-} \times \Omega$−cm to $2\ 2.24\ 10^{-} \times \Omega$-cm) and lowered the optical band gap of the films (3.64 eV to 3.57 eV), with best values at 10% Germanium concentration when annealed in nitrogen ambient. Films annealed in nitrogen had the lowest band gap of about 3.55 eV and had electrical resistivity of $2\ 5.23\ 10^{-} \times \Omega$−cm , values that offer better potential for the films when used for optoelectronic applications compared to the ones treated in the Air and Argon. Key words: Nitrogen, ambient, Germanium Composite, optical, electrical, structural

Influence of Solvents on the Electrical Parameters of Poly(2,5-Bis(3-Alkylthiophen-2-Yl)Thieno[3,2-B]Thiophene) (PBTTT) Field Effect Transistor

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In this study, we report on the effect of solvents with different boiling points on the electrical performances of poly(2,5-bis(3-alkylthiophen-2-yl)thieno[3,2-b]thiophene) (PBTTT) transistors. Three solvents have been used for PBTTT thin film processing: toluene, chlorobenzene (CB) and tetrahydrofuran (THF). The highest values of mobilities were 3.42 $\times 10^{-2}$ $cm^2 \cdot V^{-1} \cdot s^{-1}$, $1.62 \times 10^{-3} cm^2.V^{-1}.s^{-1}$ and 1.78×10^{-2} $cm^2.V^{-1}.s^{-1}$ respectively for PBTTT devices using chlorobenzene, toluene and tetrahydrofuran and heated respectively at 120°C, 150°C and 120°C. We have correlated these electrical performances with AFM images in order to point out the role of morphological properties. It is found the liquid crystalline state formation in PBTTT film from THF and toluene which drives the electrical parameters.

Keywords: PBTTT, Solvent, Temperature, Field Effect transistor.

How to Capture Solar Energy

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We have so far been limited in our capacity to harness energy from the sun due to our inability to control sunlight - solar panels require direct sunlight. Harvesting diffuse light - the kind that bounces of buildings and clouds - is in some sense 'forbidden' due to the Second Law of Thermodynamics - diffuse light is 'disordered', and 'ordering' it means we reduce the entropy of the system. We have developed novel ways around this limitation - through the use of Luminescent Solar Concentrators and carrier multiplication photophysics, using processes such as singlet fission. Singlet fission is a carrier multiplication process in organic semiconductors that generates two electron–hole pairs for each photon absorbed. Singlet fission occurs on sub-100 fs timescales with yields of up to 200%, and photovoltaic devices based on singlet fission have achieved external quantum efficiencies above 100%. The major challenge for the field is to use singlet fission to improve the efficiency of conventional inorganic solar cells, such as silicon, and to break the Shockley–Queisser limit on the efficiency of single-junction photovoltaics.

We also introduce some analysis methods to explore photoinduced charge dynamics known as SPV. We will demonstrate SPV measurements on mixed ionic-electron conductors, such as perovskites, which have previously been poorly understood. We outline a new understanding of SPV measurements, supported by experimental evidence on perovskite bilayers. Our understanding of the SPV measurement in the context of dynamic ionic motion naturally leads to avenues for the selective control of ion migration in perovskite bilayers, demonstrated here by altering the surface passivation treatment. This opens new avenues for the rational design of strategies to improve the photovoltaic properties of perovskite solar cells and LEDs.

Keywords: Photon Multiplication, Charge Dynamics, Solar Cells, Energy Harvesting

Synthesis of Cu (II) and Pd (II) Complexes Catalyst Encapsulated in a Nanoreactor

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In industrial parlance, heterogeneous catalysts are widely preferred over homogeneous catalysts for most industrial processes due to their ease of separation and recyclability[1]. The "Achille heel" faced with homogeneous catalysts is their separation difficulties from the reaction mixture, which is generally costly compared to their counterparts[1,2]. As such, one of the best ways that has been recognized is to design a novel heterogenized homogeneous catalyst (known as "hybrid" catalyst) by immobilizing a homogeneous catalyst on a solid support to improve the catalyst recovery and its recyclability. However, previous studies revealed that there is a decrease in the catalyst activity and poor recovery due to the leaching of the catalyst from the support[3]. To combat this, hollow structured carbon nanomaterial such as hollow carbon spheres (HCSs) can be used as an ideal nanomaterial for the encapsulation of the catalysts to minimize leaching and improve the catalyst activity, separation, and its recyclability. The HCSs exhibit a hollow cavity that can act as a nanoreactor to encapsulate various nanosized materials and can act as a filter to separate products from the catalyst[4].
This study reports on the encapsulation of a Schiff base Cu and Pd complexes inside the HCSs i.e., Cu-complex@HCSs and Pd-complex@HCSs. The Schiff base ligands were synthesized by a condensation reaction between salicylaldehyde and aniline. The Cu or Pd complexes were prepared by reacting the ligand and Pd or Cu source under reflux at 60 °C. HCSs were prepared by the chemical vapour deposition method, and the Cu complex@HCSs or Pd complex@HCSs were achieved through hydrothermal impregnation method. The ^{1}H NMR revealed the successful formation of the salicylaldimine ligands and Pd complexes. The IR spectra of both the Pd and Cu complex showed a shift in the characteristic peaks of salicylaldimine ligands to lower frequencies and the absence of the -OH group which suggested the formation of the complexes. TEM data revealed the formation of the HCS, and successful incorporation of the complexes as observed from the thermogravimetric analysis studies.

Keyword: Homogeneous catalyst, Hybrid catalyst, Hollow carbon spheres, Schiff base ligands, Complexes

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Nanoconfined Columnar Discotic Liquid Crystals for Microelectronics and Photovoltaic

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I will present fundamental and experimental studies of the physical properties of columnar discotic liquid crystal (CDLCs) confined in highly ordered porous templates at the nanoscale. CDLC molecule of planar shape, consist in rigid polyaromatic nuclei surrounded by functionalizable flexible aliphatic chains, and are capable of self-assembly in columns, thereby promoting overlap of their π-electron orbitals. This makes these materials real candidates for applications in molecularelectronics and photovoltaics due to the possibility of migration of the charge carriers along their columns. However, these applications require a good control of the parameters affecting the alignment mechanisms in the columnar phases of large single domains, preferably at room temperature. A very promising approach to optimize the diffusion lengths of charge carriers has been proposed, based on the formation of oriented CDLC nanowires by self-assembly in so-called"templates". However, structural and dynamical proprieties and confinement effects are still scarce,and could be a real scientific lock to their implementation. Our study is focused on commercial CDLC (HPT) and Pyrene derivative Py4CEH which are confined in porous alumina and porous silicon membranes with pore diameters of c.a. tens of nanometers. The phase diagram was first studied by DSC and more deeply characterized by neutron scattering. In confined geometries, we observe a depression of the phase transition temperatures, a broadening of the columnar phase stability domain and an opening of hysteresis loops amplified by smaller pore size. A high orientational order was found in the bulk columnar phases by solid-state NMR, and the structure of confined columnar systems, dominated by a radial distribution with homeotropic anchoring wasobserved. The molecular dynamics was studied by quasielastic neutron scattering. It is affected by confinement: large lengthscale motions are massively slowed down, whereas the rapid and local dynamics becomes submitted to large distributions of correlation times.

Keywords: Liquid crystal, discotics, porous matrix, confinement, phase, transition, structure, dynamics, anchoring, homeotropic, planar…

Plant-Based Bionanocomposites as Modifiers for TiO_2: Towards Greener Photocatalytic Processes

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The developments of photocatalysts technology is generally hindered by the extremely high temperatures used during catalyst preparation which translates to high costs in terms of energy requirements. The high temperatures stem out of the need to form crystalline semiconductors. This is despite the demonstration in several literature that amorphous semiconductors are also capable of driving efficient photocatalytic decontamination processes (Shao *et al.*, 2015; Moshoeu *et al.*, 2020). Amorphous chalcogenides can be prepared at low temperatures and, therefore, are energy efficient as photocatalysts. We hereby investigate the influence of plant-based bionanocomposites as modifiers for titania (TiO_2) composites on the physicochemical properties and the photocatalytic properties. Amorphous titania-based photocatalytic bionanocomposites were fabricated from plant based adsorptive bionanocomposites. Based on the composition of the bionanocomposites, two types of photocatalytic bionancomposutes were fabricated; one type was based on adsorptive pine-magnetite bionanocomposite (PMC) and the other on acrylic acid grafted pine magnetite composite (GAA). Since the preparation procedure for amorphous TiO_2 eliminates post-synthesis calcination, the photocatalytic bionanocmoposites were inherently doped with carbon and therefore named PMC–a-C,TiO_2 and GAA–a-C,TiO_2. The effect of co-doping the bionanocomposites was explored by addition of N as a dopant to form PMC–a-C, N,TO_2 and GAA–a-C, NTO_2. The characteristics and photocatalytic performance of the bionanocmposites were benchmarked against C, TiO_2 and C, $NTiO_2$ fabricated under similar conditions as the bionanocomposites. Doping with N and the nature of the bionanocomposites had a significant influence in the morphological and surface properties while the optical properties were shown to be independent of either factor. The synergy of GAA and N-doping had the most pronounced effect on the morphological and surface features as shown by the typical correlation between the decrease in particle size and the increase in surface area. The Photocatalytic performance was evaluated under UV light for the degradation of a dye cocktail consisting of Reactive red 120 (RR 120) and Rhodamine B (RhB), of the same concentration (25 ppm). The dye cocktail was spiked up to pH 8 using NaOH to simulate the pH conditions typical in real textile wastewater. The N doped photocatalysts and bionanocomposites (C, $NTiO_2$, PMC–a-C, N,TO_2 and GAA–a-C, NTO_2) all followed the zero order kinetics while the other bionanocomposites followed 1st order kinetics with the GAA based bionanocomposites and C,TiO_2 having the highest overall dye removal. The work has hereby demonstrated that acrylic acid capped adsorptive bionanocomposites make suitable modifiers for greener photocatalysts with a performance that is comparable to those of highly crystalline forms of doped TiO_2.

Keywords: Plant-based photocatalysts; Green photocatalysis; amorphous titania; doping

Elaboration of Bio-Inspired Parahydrophobic Nanostructured Surfaces by Electropolimerization of Thiphene-Based Monomers

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Controlling the wettability of solid surfaces is an important problem that is attracting increasing interest, both from a fundamental and a practical point of view, by adapting topography and surface chemical compositions. [1] This is how bio-inspiration has become an excellent way to break into this scientific field and this is particularly true for nano-structured surfaces. [2]
Indeed, many potential applications are expected with these materials such as self-cleaning coatings, water collection and transport systems, anti-fingerprint and optical anti-reflective, anti-bio adhesion. [3-4]
Electropolymerization is an excellent and fast process for the design of structured surfaces. It is in this context that our team, in collaboration with the NICE-Lab group, has undertaken various actions to develop nanostructured surfaces by electropolymerization, via a bio-inspired approach. The aim of this work was to develop hydrophobic materials with strong adhesion to water from thiophene-based monomers by the electrochemical method in different solvents.

Keywords: Wettability control, Hydrophobic surfaces, Electropolymerization

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Synthesis and Self-Assembly of 1D Coordination Polymers

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Metal hydroxyacetates have been shown to form 1D adducts that can *in situ* self-assemble into tunable 3D high-aspect ratio nanomaterials. This talk discusses the synthesis of p-block metal hydroxyacetate and their lanthanide homologues, illustrating the role valence shell in the structure of resulting compounds. Post synthesis ligand ablation in the latter renders the high-band gap materials colored while in the latter photochromism is lost due to enhanced absorption (band overlap).

Keywords: Carbon, electrical conductivity, ligands, materials, oxides

A Magnesium Single Crystal Complex: IR and Multinuclear NMR (^{12}Mg, ^{1}H, ^{13}C) Spectroscopic Characterized, Thermogravimetry and Uv-Visible Analysis

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The objective is to characterize the magnesium cation complex and to study the antibacterial effect of these types of complexes in medicine field. The tetrahydrated magnesium malonate complex [$^{-}$OOC$(CH_2)_2$COO^{-},Mg^{2+}.$4H_2O$] has been isolated as single crystals by using a new experimental "one pot" method from between malonic acid HOOC$(CH_2)_2$COOH, $CyNH_2$ and $MgCl_2.6H_2O$ in methanol solvent. Compound **1** was characterized by X-ray diffraction analysis, elemental analysis, IR spectroscopy, multinuclear solution NMR (^{12}Mg NMR, ^{1}H NMR, ^{13}C NMR) and thermogravimetry analysis. The asymmetric unit is one $Mg(H_2O)_4^{+}$ coordinated by one $^{-}$OOC$(CH_2)_2$COO^{-}, one oxygen atom of the oxyanion is linked with one hydrogen atom of one H_2O molecule via an intramolecular O---H hydrogen bond. In supramolecular view, the structure is tridimensional one. In the Infrared spectrum appeared the asymmetric and symmetric vibrations of carboxylate anions as strong bands and coordinated water molecules in $Mg(H_2O)_4^{2+}$ as strong and medium bands. The acid acetic form of absorption band of water molecule is corroborated with the presence of OH---O hydrogen bonds. The Thermogravimetry analysis diagram shows two main weight loss: the first pic is corresponded of water molecules loss and the second pic is the loss of organic part. This data is corroborated with the diffractometer data. The ^{12}Mg NMR data gives a single signal with a precise value showing a coordinated Mg atom. The uv-visible spectrum has appeared an hyperchrome intensity due to the Metal-ligand transfert.

Keywords: magnesium complex, spectroscopic characterized, diffractometer data, thermogravimetric analysis, ^{12}Mg NMR data, weight loss, hydrogen bonds, uv-visible analysis

Fabric-Integrated Polymeric Photonic Crystal Fibers for Textile Tracing and Sorting

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Circular supply chains in manufacturing and retail require more accurate product labelling and traceability. This is particularly desirable in the textile and apparel industries. Unfortunately, in the apparel industry, as just one example, product life cycle management is hampered in part by inaccurate, poorly readable, and detachable standard care labels. To address this problem, we seek to enable a labelling system that is integrated into the fabric itself, intrinsically recyclable, low-cost, and enables high information fidelity and rapid readout after years of normal use. The approach described here is to use all-polymer photonic crystals in the form of fibers that could be manufactured at scale and integrated seamlessly into textiles. The photonic fibers are designed using standard transfer matrix formalism and then fabricated by thermal drawing. One novel aspect of these 1DPCs is that they consist of >100 layers of polymers having low refractive index contrast ($\Delta n=0.1$) and sub-micrometer individual thickness. Nevertheless, optical stack design is described here that enables distinguishable reflectance features in the 1-5.5 µm wavelength range, which is experimentally realized and characterized using *in-situ* Fourier transform infrared spectroscopy. Drawn fibers are then integrated into multiple woven structures and further characterized by near-infrared spectroscopy and short-wave infrared imaging, techniques commonly used in industrial facilities for sorting materials. Importantly, the fibers' optical design also enables use of overtone peaks to avoid overlap with parasitic molecular absorption, substantially improving signal-to-noise ratio (and therefore ease and speed) of readout. The ability to produce kilometers of fiber that are compatible with existing textile manufacturing processes, coupled with low input material cost, make these a potential market-viable improvement over the standard care label.

Keywords: photonic crystal, polymeric fiber, textile, recycling, tracing

Synthesis of 1-D VO_2 Nanobelts for High Sensistive and Selective CH_4 Gas Sensing

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Gas sensor unquestionably plays a significant role in majority of technological sectors in the world we live in today, they are extensively utilized for public safety, pollution monitoring, quality control, air analysis, smart building and transportation, and other applications. Metal oxides (MOs) gas sensors features tremendous potential for detection of over 150 gases due to their high efficiency, easy fabrication, high sensitivity, compactness, instantaneous detection, ease to use, portability and power efficiency. Mott-type pristine and doped vanadium dioxide (VO_2) - nanobelts (NBs) with monoclinic crystalline symmetry were grown via hydrothermal method followed by thermal annealing @ 500 ° C under vacuum. VO_2 (NBs) demonstrated to be effective methane (CH_4) gas sensors. The gas sensing response of the devices were examined by monitoring variation electrical resistance via KSGAS6 S gas sensing station. The material optimal temperature for target gas response measurements were conducted, followed by response analysis towards different gas concentration. Fabricated pristine and doped VO_2 (NBs) were characterized by X-ray diffraction, electron microscopy (SEM and TEM) equipped with energy dispersive x-ray spectroscopy (EDS), X-ray photoelectron spectroscopy (XPS). The nanobelts (ultralong belt-like) nanostructures could be an ideal system for fully understanding dimensionally confined transport phenomena in functional oxides and for building functional devices based on individual nanobelts structures.

Keywords: Hydrothermal process; Methane (CH_4); Vanadium dioxide nanobelts (NBs); Semiconductor metal oxide; Gas sensor

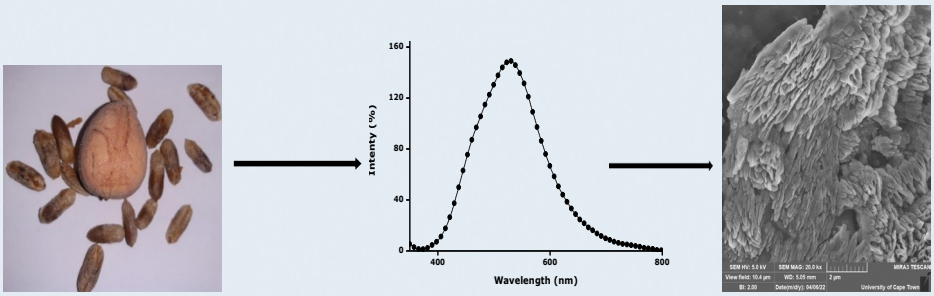
Green Synthesis of Metal Sulphide Nanoparticles: Morphological, Chemical, and Optical Properties

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Metal sulphide nanomaterials have attracted great attention because of their excellent properties. They have been studied and investigated for use in batteries, catalysts, light emitting diodes, solar cells, and many other fields currently they are also being studied in Agriculture as nanofertilizers. This is mainly due to the fact that sulphur is one of the essential nutrients for plants and metal sulphides are known for their anti-microbial and anti-bacterial activities. Transition metals have interesting chemical and physical properties. They are able to undergo different reactions because of their various oxidation states 0, +1, +2, +3 etc. Due to those unique characteristics and properties, the metal-based nanomaterials have gained attention in many nanotechnology applications. Some have been discovered to be safe inorganic materials because of their less-toxicity with antifungal activity, and remarkable potential in a wide range of biological, catalytic and other applications especially in the form of nanoparticles. Metal sulphide nanostructures have been synthesized by a variety of chemical or physical methods. Currently, there has been an increased emphasis on the topic of "green" chemistry and chemical processes. Environmentally benign reducing agents and nontoxic solvent media are some of the key issues that merit significant consideration in a green synthetic strategy. In this study metal sulphide nanoparticles were synthesized through the green route. Avocado and date seeds were used as reducing agents. Optical properties of the nanoparticles were studied using UV-Vis, photoluminescence, diffuse reflectance, and characterized using SEM, TEM, XRD, and FTIR.



Keywords: Metal Sulphide, nanomaterials, green synthesis

Nanoscale Insights on Sepia Melanin Structure for Sustainable Organic Electronics

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Eumelanin is the black-brown pigment belonging to the melanin family, ubiquitous in flora and fauna. The pigment is an electro-active material: it conducts both ionic and electronic charge carriers. Therefore, it is a potential candidate for organic electronic devices and their powering elements (e.g., transistors, sensors, supercapacitors). Being abundant in nature and biodegradable [1], eumelanin is a prototypical material for sustainable organic electronics. Sepia melanin (i.e., the bio-sourced eumelanin extracted from the ink sac of the cuttlefish Sepia Officinalis) features a spherical-like granular structure with a granule size ranging between 100 and 200 nm [2,3]. The high electronic conductivity recently reported in printed films of Sepia melanin [4] encouraged us to study its nanoscale structure to understand the electronic transport mechanisms. In this work, we fabricated Sepia melanin films using drop-cast, electrochemical and Langmuir Blodgett deposition methods. High-resolution Atomic Force Microscopy (AFM) shows intimate contact between granules enabling intergranular conductivity. Furthermore, conductive-AFM and scanning tunneling microscopy (STM) reveal the possible presence of subunit particles (diameter about 10 – 50 nm), expected to be electronically conductive. Our study provides insights into the nanoscale electronic conductivity towards a well-established transport physics in devices using eumelanin as a bio-sourced active material.

Keywords: melanin, nanostructure, electronic conductivity, sustainable electronics.

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Using the Ferh System to Thermally Control the Magnetic Field Generated by the FePt System

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Abstract: Nowadays, Micro-Electro-Mechanical Systems can be incorporated into a wide variety of applications. The optimization of their performance mainly relies on the choice of their activation type. The most common ones are electrostatic, piezoelectric, thermal, magnetostrictive or magnetic. Benefiting from the advantages of microelectronic manufacturing processes, electrostatic actuation remains the most widely used. At equivalent volume, the energy densities that can be transformed within an electromagnetic system are several orders of magnitude higher than those of a purely electrostatic system. However, magnetic or electromagnetic micro-systems also present challenges in terms of production of efficient magnets and integration processes at the required dimensions. Furthermore, as the size of microsystems decreases, purely magnetic actuation may be preferred to electromagnetic actuation based on coil and magnet interactions. To address this goal, we have opted for an original approach that consists in using the temperature induced antiferromagnetic-ferromagnetic transition of the FeRh system to shunt the magnetic stray field created by arrays of FePt micro-magnets. FePt-FeRh bilayers were deposited on pre-patterned Si substrates and their behavior was analyzed on the basis of magnetic measurements and magneto-optical observations using uniaxial magneto-optical indicator films. The results show the feasibility of a hybrid film structure with both FePt and FeRh properties, which exhibits a short-circuiting effect of the flux lines produced by FePt depending on whether the FeRh is in its ferromagnetic or antiferromagnetic state.

Keywords: Magnetic Microsystems Activation, Thermally Switchable Magnetic Films, Magnetic Materials

Comparative Investigation of the Infrared Spectrum of Achiral Single-Walled Boron Nitride Nanotubes.

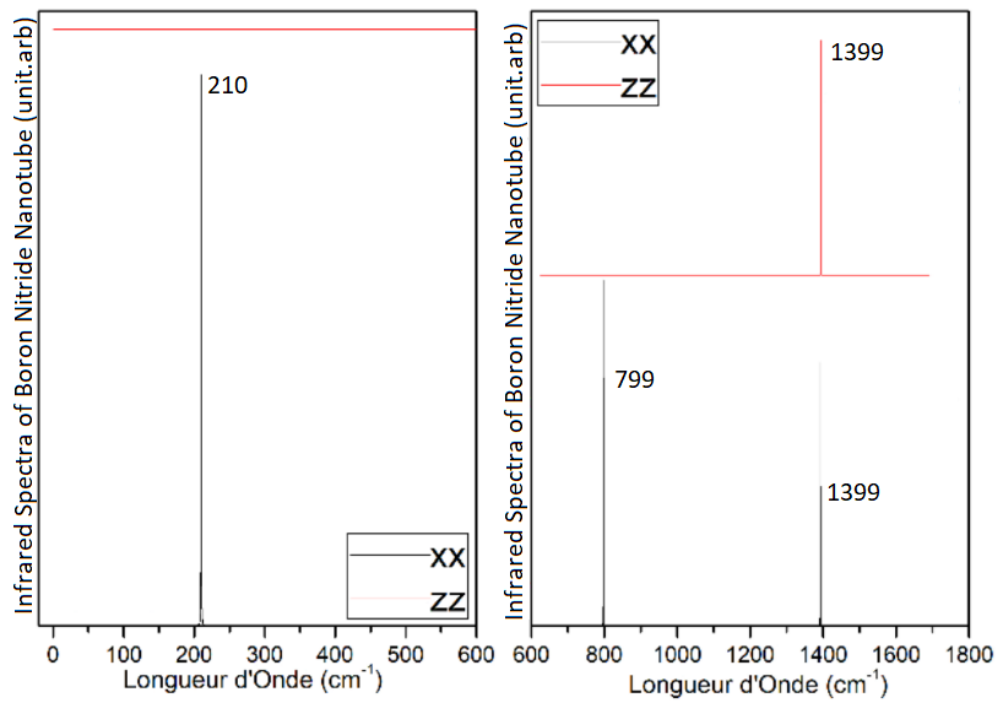
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The comparative investigation of the achiral single-walled boron nitride has been performed by using the spectral moment's method and the infrared spectra of single-walled boron nitride nanotubes are calculated. The dependence of these modes was computed according to the chirality, diameter and length of the nanotube. These forecasts are useful to understand the experimental infrared spectra of boron nitride nanotubes.

Preliminary Results



Schottky Diodes and Perovskite Solar Cells Fabricated from Cerium Doped Copper Oxide Prepared by Spin Coated Assisted Sol Gel Method

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In this work, we investigated the synthesis, characterization and application of pristine copper oxide (CuO) and CuO doped with cerium (Ce) (1, 2, 3, and 4 wt%) using spin coating assisted sol gel method. X-ray diffraction patterns confirmed the monoclinic CuO crystal structure with c2c space group. Raman spectroscopy studies revealed the Ag, and Bg vibrational phonon modes for both the pristine and doped CuO samples. Scanning electron micrographs of the thin films revealed nanoparticles that were well dispersed on the surface with a decrease of grain size with increasing dopant concentrations. UV-vis spectra showed little absorption in the visible region and increase in the absorption of UV light with increase doping concentration up to 3wt%. Density function theory (DFT) was used to simulate optical absorption and conductivity using CASTEP and the simulated absorption spectra were in good agreement with the experimental. CuO Schottky diodes (SD) were fabricated with gold (Au) as the Schottky contact and aluminum (Al) as Ohmic contact and dark current-voltage (*I-V*) measurements were conducted. Pristine and doped CuO-SDs both rectified, and the forward and reverse *I-V* characteristics of the Ce-doped devices differed by three orders of magnitude and those of pristine CuO film by two orders of magnitude. Moreover, the Schottky barrier height increased as Ce doping centration increased. Pristine CuO device had an ideality factor of 2.526 which decreased the most to 1.019 for 1 wt% Ce doped CuO device. The effect of Ce doped CuO as hole transport layer (HTL) for perovskite solar cell (PSC) were also investigated. Our findings indicated that the PSC with 3wt% Ce-doped CuO as HTL had a best performance.

Keywords: CuO, Schottky diode, perovskite solar cell, DFT, electrical properties

Analysis of the Structure and Surface Properties of Biosynthesized Yttria Nanoparticles

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Nanoparticle biosynthesis using plant precursors is currently of great interest due to its simplicity, environmental friendliness, and low cost compared to other nanoparticle synthesis methods... However, yttria has received little attention. It is one of the most promising rare earth materials that can be used in ceramic superconductors, electronics, and light-emitting materials. This presentation reports biosynthesis and characterization by XRD, Raman scattering, and Fourier Transform Infrared (FTIR) spectroscopy. The samples were annealed for 2 hours each at 300, 400, and 500°C for 2 h. Annealing temperature affects the composition, size, and lattice constant of yttria. It is noted that impure yttria forms around 300 °C. The recovery of pure yttria is facilitated by raising the annealing temperature to 400–500 °C. The average size of the nanoparticles for annealing at 300, 400, and 500 °C, respectively, was computed and determined to be 20, 40, and 30 nm. This shift in nanoparticle size is attributed to the material's recrystallization as a result of the removal of impurities from the samples. As the annealing temperature rises, the average lattice parameter tends to get closer to the reference value. Raman's analysis validates XRD results. The FTIR analysis confirms the formation of yttria and shows that exposure to ambient air directly affects the surface state of yttria nanoparticles through the absorption of atmospheric CO_2 and H_2O, with the latter effect being strongly dependent on the purity of the synthesized yttria.

Keywords: Nanoparticles, biosynthesis, yttria, XRD, Raman, and FTIR

Producing Multiple Qubits via Spontaneous Parametric Down-Conversion

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We have designed Gaussian masks to subdivide the pump beam before passing it through a BBO. In this way, present an approach to possibly produce multiple entangled photon pairs through spontaneous parametric down-conversion (SPDC).

Performance Evaluation of Bi_2O_3@GO and Bi_2O_3@rGO Composites Electrode for Supercapacitor Application

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Among other energy storage systems, supercapacitors have been of higher research interest for optimal energy utilization due to their outstanding intrinsic properties such as; high electrical response, great durability, a wide range of operating temperature and voltage. In this work, synthesis and comparison of the electrochemical performances of graphene oxide doped with Bismuth oxide (Bi_2O_3@GO) and reduced graphene oxide doped with Bismuth oxide (Bi_2O_3@rGO) without any binder material were carried out using a very low concentration (1.0 M) of KOH electrolyte, the solvothermal method of nanomaterial synthesis was employed. The produced materials were studied using X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FT-IR), and electrochemical characterizations. An improved performance was recorded by the electrode made of Bi_2O_3@rGO which achieved; 560 Fg^{-1} specific capacitance at 5 mVs^{-1} scan rate, 280 $Whkg^{-1}$ and 40 $kWkg^{-1}$ energy and power densities respectively, the electrode also retained 99% of its capacitance after 3000 galvanostatic charge-discharge (GCD) cycles.

Keywords: Bismuth oxide; Graphene oxide; Composite; Electrochemistry; Supercapacitor

Fast Ion-Conducting Glass Nanofibers for All-Solid-State Batteries

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The rising concentration of combustion driven vehicles in urban areas poses serious threats to human health by pollution from nitrogen oxides and micro- or nanoparticles known as particulate matter (PM). Long-term exposure to these toxic substances has been linked to serious health problems, such as depression, diabetes, dementia, Alzheimer's and Parkinson's. Legislation and the increasing demand for more ecological cars have persuaded many car producers to focus on the development of a new generation of electric vehicles (EV) that have the potential to replace diesel and petrol cars. Such cars must be competitive in terms of driving range, energy charging rate, fire safety and price. The main drawback is that current Li-ion battery cells, based on carbon anode materials and liquid electrolytes, are unable to achieve sufficiently high energy density, safety and cost effectivity. Therefore, we present a new type of high capacity all-solid-state Li battery in which the carbon anode and liquid electrolyte are substituted with glass nanofiber composites. For the composites, the amorphous glass nanofibers and nanoparticles were structured to form gradient functional layers exhibiting high surface-to-volume ratios yielding a high surface conductivity. For the nanofibers, we prepared fast ion-conducting (FIC) glasses in a $LiCl$-Li_2O-P_2O_5-(B_2O_3-Fe_2O_3-V_2O_5-MoO_3-WO_3) system and formed them to nanofibers using the electrospinning. Using electrochemical impedance spectroscopy and chronoamperometry, the surface ionic and electronic conductivities were determined. The prepared precursors and final composites were also characterized using optical and electron microscopy, simultaneous thermal analysis, infrared and Raman spectroscopy, and nuclear magnetic resonance. The effects of the composition and preparation procedure on the electrochemical properties of the nanocomposites and their performance in the battery cell are discussed. Collectively, our results indicate that the developed FIC glass nanofiber composites have potential for the construction of high-capacity all-solid-state batteries to power plug-in electric cars.

Keywords: glass, nanofibers, all-solid-state battery



POSTER
PRESENTERS

Magnetite Functionalized Nigella Sativa Seeds for the Uptake of Chromium (Vi) and Lead (Ii) Ions from Synthetic Wastewater

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The aim of the present study was to utilise pristine and magnetite-sucrose functionalized *Nigella Sativa* seeds as the adsorbents for the uptake of chromium(VI) and lead(II) ions from synthetic wastewater. Pristine *Nigella Sativa* seeds were labelled (PNS) and magnetite-sucrose functionalized *Nigella Sativa* seeds (FNS). The PNS and FNS composites were characterized by Fourier transform infrared spectroscopy (FTIR) and X-ray powder diffraction (XRD). The FTIR analysis of both adsorbents revealed the presence of vibrations assigned to 1749 and 1739 cm^{-1} (-C=O) for ketonic group for both adsorbents. The amide (-NH) peak was observed at 1533 and 1527 cm^{-1} on FNS and PNS composites, respectively, whilst the carboxyl group (-COOH) were observed at 1408 cm^{-1} on both adsorbents. The XRD results of FNS and PNS composites showed a combination of spinel structure and *y*-Fe_2O_3 phase confirming the formation of iron oxide. The influence of operational conditions such as initial concentration, temperature, pH, and contact time was determined in batch adsorption system. The kinetic data of Cr(VI) and Pb(II) ions on both adsorbents was described by pseudo-first-order (PFO) model which suggested physisorption process. The sorption rate of Cr(VI) ions was quicker, it attained equilibrium in 20 min, and the rate of Pb(II) ions was slow in 90 min. Freundlich isotherm described the mechanism of Pb(II) ions adsorption on PNS and FNS composites. Langmuir best fitted the uptake of Cr(VI) ions on PNS and FNS. The results for both adsorbents showed that the removal uptake of Pb(II) ions increased when the initial concentration was increased; however, Cr(VI) uptake decreased when the initial concentration increased. The adsorption of Cr(VI) and Pb(II) ions on both adsorbents increased with temperature.

Keywords: Functionalized, Pristine, *Nigella Sativa*, Magnetite and Sucrose

Thermal Decomposition of Copper Acetate at Various Temperature and Time to Form Copper Oxide/ Copper Nanoparticles

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Copper acetate is preferred as precursor to synthesis copper oxide nanoparticles. Copper oxide and copper nanoparticles were prepared by thermal decomposition of solid phase copper acetate at various time (1-3) hrs and temperature (200-500) °C. The method is simple, less expensive, avoid toxic solvent, and avoid use of passivating agents. The FT-IR show that calcined copper acetate monohydrate shows major changes in absorption peaks associated with methyl, carbon-oxygen double bond, carbon-oxygen single bond, and copper-oxygen bond functional groups. Thermogravimetry show that copper acetate monohydrate decomposes at about 250 °C to form copper. The TEM images show a combination of shapes which includes icosahedrons, truncated cubes, and nano-whiskers made from sphere with diameter of 7.43-0.83 nm.

Keywords: Copper acetate ($CuAc_2.H_2O$), coper oxide, copper, temperature, time, nanoparticles.

Green Synthesis and Characterization of Iron Oxide and Silver Nano Particles Prepared from Colophospermum Mopane Aqueous Leaf Extract

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Nowadays, green methods for nanoparticles synthesis, which is eco-friendly, hazard free, cost-effective, and easy is gaining recognition, acceptance and appreciation by researchers. This has led to recent shift of focus from the conventional methods of chemical synthesis which involves toxic solvents, hazardous chemicals, high energy and time consuming. Synthesis of Iron Oxide and Silver Np's from precursor solutions of $FeCl_3 .6H_2O$ and $AgNO_3$ respectively with *colophospermum mopane* aqueous leaves extract given code 'A' was successfully afforded in this research. The extract act as a reducing, stabilizing and capping agent in this synthesis procedure. The green synthesized nanoparticles were characterized using various techniques being ultraviolet-visible spectroscopy (UV-VIS), Fourier transform infrared (FTIR), powder X-ray diffraction (XRD), scanning electron microscopy (SEM), visual inspection and magnetic attraction for the Iron NP's. The UV-VIS showed absorption peaks characteristic to surface plasmonic resonance for the synthesized NPs. Functional groups in the phytochemicals of biomolecules responsible for the reduction process were determined by FTIR. The immediate colour changes from light brown to dark colours in reaction mixtures upon mixing the precursor salt solutions and leaf extracts confirmed the formation of the nanoparticles in each case.

Keywords: Green synthesis, Sliver Nanoparticles, iron nanoparticles, *Colophospermum mopane*, Biomolecules.

Elaboration and Characterization of Ceramic-Type Perovskite Nanoparticle Solar Cell Deposited on Ito Glass Substrates

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The objective of this work is to develop and characterize solar cells based on ceramic type perovskites composed of $LiFePO_4$ from NPK fertilizer deposited on ITO (indium tin oxide) glass substrates. NPK fertilizer is an inorganic material that is very abundant in Senegal and which is used for gardening. The ceramics which are used in the context of this thesis are in the state of powder at the beginning, dried at 100°C in an oven in the form of powders. Then these powders are baked at 800°C (B) and 900°C (A) dispersed in a cola cordifolia biopolymer for the deposits of perovskite layers of first four samples. These powders are ground, sintered at 1000°C for the last four.
In this work, we developed thin layers on an ITO/TiO_2 substrate with NPK-type perovskite nanoparticles ($LiFePO_4$) dispersed in a biopolymer acting as a matrix, depending on the annealing temperatures and we also interested in the morphological characterization with optical microscopy to see the morphology and the dispersion of seeds. Scanning electron microscopy (SEM) images, allowed use to see that there is a fairly homogeneous distribution of nanoparticles and retains their crystalline form. The development of different thin layer has enabled us to make solar cells. Finally, the current voltage (I-V) measurements are carried out under shade and under light in order to extract the various cell parameters and to evaluate their performance.

Keywords: solar cells, NPK ceramics, Cola cordifolia, thin films, perovskites.

Tungsten Oxide Thin Film for Room Temperature Nitrogen Dioxide Gas Sensing

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Tungsten oxide (WO_3) thin films for gas sensing have been successfully deposited using reactive direct current (DC) magnetron sputtering at different deposition temperatures (300 ºC, 400 ºC and 500 ºC). The structural, morphological properties, thickness and composition have been investigated using X-ray diffraction (XRD), scanning electron microscopy (SEM) and Rutherford backscattering spectrometry (RBS) techniques. To investigate the effect of deposition temperature on the gas sensing properties of deposited thin films on alumina substrates was conducted using the Kenosistec gas sensing unit. WO_3 thin film deposited at 500 ºC exhibited a higher response when sensing Nitrogen dioxide (NO_2) at room temperature as compared to the thin films prepared at 300 ºC and 400 ºC, respectively. However, as deposited WO_3 thin films exhibited low sensitivity when sensing reducing gases such as hydrogen (H_2) and ammonia (NH_3), which was an indication of good selectivity properties of WO_3 related sensors.

Keywords: Tungsten Oxide, DC Reactive Sputtering, Thin Films, Nitrogen Dioxide, Gas Sensing

Electrospinning PVDF – Some of the Challenges

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Properties such as piezoelectricity, lightweight, high thermal stability, abrasion resistance and chemical resistance make polyvinylidene fluoride an excellent candidate for diverse applications.[1] PVDF nanofibers have been extensively investigated to gather insight into the advantages of using these fibers in its applications.[2] Electrospinning provides one of the easy routes to fabricate nanofibers. Our efforts to produce PVDF nanofibers ran into unexpected challenges. Beadless fibers were eventually obtained when DMF/acetone solvent mixture was used to make the polymer solution, along with appropriate salt and surfactants. The presentation will focus on the challenges encountered and how it can be addressed when electrospinning PVDF.

Keywords: PVDF, electrospinning, nanofibers

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Biosynthesis and Photocatalytic Studies Adansonia Digitata Leaves' Mediated TiO_2 Nanoparticles

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High purity Titanium dioxide TiO_2 nanoparticles are bio-synthesized for the first time via a natural extract of the African indigenous Adansonia digitata leaves. The nanoparticles are thermally oxidized in the air for 2 hours at annealing temperatures of 700, 800, and 900°C. Subsequently, the nanoparticles are characterized for their functional group's identification, morphological and optical properties. The XRD patterns showed well-defined peaks of anatase and rutile phases, while the FTIR revealed peaks at 498 and 753 cm-1 assigned to vibrational modes of the Ti-O and the Ti-OTi groups respectively. TEM analysis revealed spherical shape nanoparticles with averaged grain sizes estimated as 3.94, 29.15, and 45.4 nm for TiO_2_700, TiO_2_800, and TiO_2 _900°C respectively. Furthermore, the Adansonia digitata leaves assisted TiO_2 nanoparticles showed an excellent photodegradation ability of 92 % towards methylene blue dye within120 minutes.

Keywords: Photocatalytic Activity; Biosynthesis; Titanium Dioxide Nanoparticles; Adansonia Digitata; Leaves Extract

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Nucleophilic Grafting, The Cathode of Cv A Nucleophile In Reactions With Halo- And Pseudo-Halosilanes

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Silylation of materials is a highly researched and widely studied specific modification of surfaces of many materials, for many reasons from applications such as modern technology and research like chemical and biological sensors [1], light-emitting devices [2], microelectronics and molecular electronics [3], corrosion protection and microanalysis [4]. Since such silylation mostly requires the presence of active hydrogen (–OH, –NH and –SH) on the surface of the material, carbonaceous substrates (CV, graphite, HOPG, CNT) are therefore the least used for this process. silylation [5]. Thus, Gelset, the industry leader in surface silylation, recently published a list of materials ranked according to their ease of silylation [5]. In this ranking, carbon (– fullerenes, graphene, CNT, carbon nano-ions etc) is the most difficult material to silylate, despite its importance in modern technologies. This problem comes from the fact that classical silylation relies on the immobilization of silyl groups by Si–O–C, Si–N–C or Si–S–C bridges which are sensitive to bases and F^- ions [6]. Thus, we show the phenomenon of grafting of various silyl groups ($VinMe_2Si$–, Ph_2SiCl–, Et_3Si–, Ph_3Si–, $(EtO)_2MeSi$–, $(EtO)_3Si$–, $(EtO)Ph_2Si$–) on vitreous carbon (CV) supports. By reduction of CV surfaces, we obtained polynucleophilic surfaces whose active sites are silicophiles. These sites are silicophiles attack the silicon atoms of the halo- and pseudohalosilanes following an S_N2 substitution. The modification of the surface of CV was made according to a covalent functionalization, this one is carried out by the immobilization of a new chemical function on the surface of the CV. The grafted electrodes were characterized by different techniques in order to confirm the presence of silyl groups on their surface. The characterization of these grafted surfaces was made by voltammperometric oxidation of ferrocene or parachloranil, SEM, EDS after bromination (in the case of Me_2VinSi–), EIS and FTIR spectroscopy. From this grafting technique, CV materials can now become one of the most favorable carriers for surface silylation. The CV is thus the subject of particular attention in various fields such as microelectronics, modern analysis, etc. This is due to the efficiency of our method, nucleophilic grafting.

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On the Selective Gamma-ray ionization of vanadium oxides: Towards the Formation of VO_2

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In this study, we report on the valence control of vanadium oxidation states towards stabilization VO_2 thin films. X-ray Diffraction measurements show that up to 300 kGy of gamma-ray radiation; the VO_2 phase remains monoclinic, crystallite size only varying slightly with the dose. X-ray Photoemission Spectroscopy shows the presence of three oxide phases (VO_2, V_2O_3 and V_2O_5) on the samples. A decrease in the oxidation states of V^{3+} and V^{5+} and an increase in the valence state V^{4+} are observed for irradiations up to 300 kGy, which favors, the vanadium dioxide VO_2 formation.

Keywords: Vanadium oxides, gamma-ray irradiation, structural properties, CubeSats, thermal shielding

Impact of the gamma-ray irradiation on the microstructure of vanadium dioxide layers as intelligent coatings for passive energy management

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Vanadium dioxide has significant thermochromic properties, reversible Metal Insulator Phase Transition (MIT), lowest transition temperature (Tt) at 68 °C, good thermal stability, drastic change in its IR transmittance then, a good candidate for <<intelligent>> passive energy coating management. The development of micro and picosatellites requires new devices for the protection of the spacecraft against temperature variations, depending on the satellite in orbit, either it is exposed to the sun or is in the shadow of the earth. These new devices do not meet the mass, surface and electrical power requirements of miniature satellites. A passive thermochromic device such as the VO_2 could provide this protective function. However, for an efficient use of this type of coating in the space domain, it is essential to study the impact of gamma irradiation on the high crystalline quality and the optical properties of VO_2. The nanostructured thin films are not modified and the material has a good crystalline quality with a monoclinic phase structure. While the phase transition is complete at this temperature, this indicates that the irradiation dose does not influence the transition of these samples. Furthermore the microstructure is modified with a slight variation of the structure. In order to understand the mechanism that governs this modification, the evolution of the crystallites size on the (100) and (011) growth planes is evaluated.

Keywords: thin film, vanadium dioxide, crystallite seeds, microstructure, smart coatings.



SYMPOSIUM-07
COMPUTATIONAL **MATERIALS SCIENCE** AND **ENGINEERING**



KEYNOTE SPEAKERS



Dr. Bagayoko *is a fellow of the National Society of Black Physicists (NSBP) and of the American Physical Society (APS). He earned the BS degree in Physics and Chemistry from the Ecole Normale Supérieure (ENSup) of Bamako, Mali, the MS in Physics from Lehigh University, Bethlehem, Pennsylvania, and the Ph.D. in condensed matter theory from Louisiana State University (LSU), under the supervision of the late Boyd Professor Joseph Callaway. Dr. Bagayoko's US Presidential Award for Excellence in Science, Mathematics, and Engineering Mentoring (US-PAESMEM) (1996), Benjamin Banneker Legacy Award (2007), and Lifetime Mentor Award of the American Association for the Advancement of Science (AAAS) partly attest to his contributions to broadening the participation of minorities in science, technology, engineering, and mathematics (STEM). With over 200 publications, over 135 of which are in theoretical physics and 65 in teaching, mentoring, and learning (TML), Dr. Bagayoko demonstrated the scholarly productivity that behooves an Honors College Dean. His superior grantsmanship is buttressed by over 80 sponsored projects whose total funding is over $62 Million, from 1985 to 2018. Dr. Bagayoko has served as consultant for national and international organizations that include the National Science Foundation, the US Department of Defense, the United Nations Educational, Scientific, and Cultural Organization (UNESCO), the United Nations Development Program (UNDP), the TOKTEN Project, and tens of universities, in and outside the US. His more than 550 local, state, national, and international presentations partly attest to his national stature as a scholar, teacher, and mentor. His successful six-year chairmanship of the Department of Physics (2009-2012) and that of Mathematics and Physics (2012-15) and four-year deanship of the Dolores Margaret Richard Spikes Honors College partly underscore his administrative prowess, besides the flawless management of over 80 sponsored projects; his execution of the total budget of $62 Million for these projects did not lead to a single audit finding. During his short tenure as the Director of the Office of Grants, Sponsored Programs, and Faculty Development (1987-1988), Dr. Bagayoko uplifted SUBR from being among the least funded universities in the competition for the Board of Regents Support Fund (BORSF) to the top two, in gross funding, and to the No. 1 position in funding level normalized with respect to the size of the faculty. Bagayoko was the principal author of the proposal and strategic plan, which passed rigorous reviews by out-of-state experts for the Board of Regents, for the establishment of the Ph.D. degree program in Science and Mathematics Education at SUBR. The more than 300 former undergraduate mentees of Dr. Bagayoko, through the Timbuktu Academy and LS-LAMP, include 22, 13, and 7 Ph.D. degree holders in Physics, Chemistry, and Engineering and 14 Student Grand Marshals. For more information, please see www.subr.edu/timbuktuAcademy and www.subr.edu/lslamp.*

Realizing the Potentials of Density Functional Theory (DFT) and of the Materials Genome Initiative (MGI)

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In 1964, Hohenberg and Kohn introduced density functional theory (DFT). In 1965, Kohn and Sham presented the local density approximation (LDA) of DFT. For more than five (5) decades, DFT has been, by far, the leading theory in describing the electronic energies and related properties of materials, from atoms, molecules, and clusters to nanostructures, semiconductors, insulators, and metals. Except for metals, however, most ab initio DFT calculations have seriously underestimated the energy gaps of finite systems (atoms, molecules, and clusters) and the band gaps of crystalline semiconductors and insulators. This *"band gap problem"* was well noted in the Nobel lecture of Professor Kohn in 1998. Some other limitations of DFT calculations, i.e., the inability to produce measured dielectric functions, optical properties, densities of states, and effective masses, are linked to the *"band gap problem."*
A brief review of the seminal article by Hohenberg and Kohn leads to two conditions that have to be met by electronic structure calculations, in order for their results to possess the full, physical content of DFT. They are (a) keeping the number of particles constant, as per the first theorem of DFT, and (b) verifiably reaching the absolute minima of the occupied energies, as per the second theorem. *Hence, results from calculations that do not meet these conditions do not necessarily represent DFT findings*. Indeed, for over five (5) decades, most DFT calculations employed a single basis set to perform self-consistent calculations; these calculations converged to a stationary state, among an infinite number of such states, mistaken for the ground state. We illustrate this fact with over 3**00** DFT calculated band gaps that are much smaller than corresponding, measured ones; in contradistinction, we list our calculations that strictly adhered to the aforementioned conditions and whose results are in excellent agreement with experiment. *We accurately predicted properties of four (4) semiconductors!* We describe our mathematically rigorous, computational method [AIP Advances 4, 127104 (2014), http://dx.doi.org/10.1063/1.4903408] that follows the correct understanding of DFT and that completes DFT in practice - *by providing the process for reaching the ground state*. In doing so, it invokes neither the self-interaction correction, nor the derivative discontinuity; the latter cannot apply to a solution of the Kohn-Sham equation! *Our method leads to the realization of the potential of DFT and paves the way for the attainment of the objectives of the Materials Genome Initiative (MGI).* In particular, this paradigm shift will (a) provide accurate descriptions and predictions of material properties to inform and to guide the design and fabrication of devices, (b) fuel the search for novel materials with desired properties, (c) advance significantly our understanding of superconductors and magnetic materials, and (d) permit the search for special nuclei using the nuclear density functional theory (NDFT).

Acknowledgments: This work was funded in part by the National Science Foundation (NSF) and the Louisiana Board of Regents, through LASiGMA [Award Nos. EPS- 1003897, NSF (2010-15)-RII-SUBR] and NSF HRD-1002541, the US Department of Energy – National, Nuclear Security Administration (NNSA) (Award Nos. DE-NA0001861 and DE- NA0002630), the Department of the Navy, Office of Naval Research (ONR, N00014-04-1-0587), LaSPACE, and LONI-SUBR. The latter funded Bagayoko's participation in this 11th A-MRS conference in Dakar.



Gian-Marco Rignanese *received his Engineering degree from the Université catholique de Louvain in 1994 and Ph.D. in Applied Sciences from the Université catholique de Louvain in 1998. During his Ph.D., he also worked as a Software Development Consultant for the PATP (Parallel Application Technology Project) collaboration between CRAY RESEARCH and Ecole Polytechnique Fédérale de Lausanne (EPFL) in the group of Prof. Roberto Car. He carried his postdoctoral research at the University of California at Berkeley in the group of Prof. Steven Louie. In 2003, he obtained a permanent position at the Université catholique de Louvain where is now part-time Full Professor, and at the F.R.S.-FNRS where he is now Research Director. Since 2022, he is also Associate Professor at the Northwestern Polytechnical University at Xi'an (China). He plays an active role in the development of different softwares (Abinit, Abipy, PyMatGen, FireWorks) and pseudopotentials through the PseudoDojo. He contributes to the Materials Project and is one of the key players of OPTIMADE consortium. More recently, he has introduced the MODNet machine-learning model for the prediction of materials properties. In 2019, he was named APS Fellow for original efforts developing free license software in the field of electronic structure calculations, and high-throughput calculations in a broad range of materials types.*

Combining the Power of High-Throughput Ab Initio Calculations and Machine Learning Towards Materials Informatics

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The progress in first-principles simulation codes and supercomputing capabilities have given birth to the so-called high-throughput (HT) ab initio approach, thus allowing for the identification of many new compounds for a variety of applications (e.g. lithium battery and photovoltaic). As a result, a number of databases have also become available online, providing access to various properties of materials, mainly ground-state though. Indeed, for more complex properties (e.g., linear or higher-order responses), the HT approach is still out of reach because of the required CPU time. To overcome this limitation, machine learning approaches have recently attracted much attention in the framework of materials design. In this talk, I will review recent progress in the emerging field of materials informatics. I will briefly introduce the OPTIMADE API that was developed for searching the leading materials databases (such as AFLOW, the Materials Cloud, the Materials Project, NOMAD, OQMD, ...) using the same queries. I will introduce the MODNet framework and its recent developments for predicting materials properties. This approach, which is particularly well suited for limited datasets, relies on a feedforward neural network and the selection of physically meaningful features. Finally, I will illustrate the power of materials informatics, combining high-throughput ab initio calculations and machine learning, through a few recent example



Ismaila Dabo is an Associate Professor in the Department of Materials Science and Engineering at Penn State University with joint appointments in the Penn State Institutes of Energy and the Environment, and in the Penn State Materials Research Institute. He received a B.Sc. in Mechanical Engineering from Ecole Polytechnique (France) and a Ph.D. in Materials Science and Engineering from MIT under the supervision of Nicola Marzari. His recent awards include the Wilson Teaching Excellence Award (2021), Materials Science and Engineering Faculty of the Year Award (2021), Corning Chair in Materials Science and Engineering (2020). He currently serves on the editorial board of the journals Computational Materials Science (Elsevier) and Science (AAAS).

First-Principles Optimization and Discovery of Materials for Energy Conversion and Storage

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Materials innovations require considerable time and resources. This presentation will discuss the use of first-principles modeling for optimizing the properties of newly synthesized (nano)materials over relevant time and length scales and for narrowing down the choice of candidate materials for target applications. The focus will be on producing hydrogen fuels photocatalytically by cleaving water molecules under solar illumination [1] and on minimizing heat transport in thermoelectric semiconductors [2]. A critical overview of Hubbard-corrected density-functional theory methods to predict band gaps and band offsets will be given, and progress in overcoming the length-scale limits of electronic-structure calculations in describing ballistic phonon transport in nanostructured semiconductors will be highlighted.

Keywords: Photocatalysis, Water Splitting, Thermoelectrics, Heat Transport, Materials Modeling

Reference

*[1] Xiong et al., Optimizing accuracy and efficacy in data-driven materials discovery for the solar production of hydrogen, Energy & Environmental Science **14**, 2335-2348 (2021).*
*[2] Chen et al., Achieving minimal heat conductivity by ballistic confinement in phononic metalattices, American Chemical Society (ACS) Nano **14**, 4235-43 (2020).*



EARLY CAREERS- SPEAKERS



Dr. Caroline Rosemyya Kwawu *is a Senior Lecturer at the Department of Chemistry, Kwame Nkrumah University of Science and Technology (KNUST) - Ghana, who specializes in the area of Physical/Theoretical/Computational Materials Chemistry. Dr. Kwawu holds a Ph.D. in Computational Chemistry from the Department of Chemistry, KNUST, supported by the Royal Society-Leverhulme Africa Award. Dr. Kwawu prior obtained a BSc. Chemistry degree with distinction in the First-Class division from the same department. She was a Visiting Scientist at the 2022 71st Lindau Nobel Laureates Meeting in Germany. Dr. Kwawu is an awardee of prestigious awards i.e., The World Academy of Sciences Grants for Individual and Collaborative Research. As well as the Royal Society Leverhulme Africa Postdoctoral Fellowship, 2018. Her research focuses on coordination materials and reticular chemistry. Using organic/inorganic materials for waste (CO2, biomass, and solar) upgrade into useful commodities, to address issues of climate change, energy scarcity (i.e., energy generation and storage technologies), health, and environmental sustainability, by providing insights into chemical processes occurring in these environments. Her research explores heterogeneous processes like surface diffusion, drug delivery, chemical decomposition, charge transfer processes, and reaction mechanisms at the atomic/molecular level. She employs DFT equilibrium, molecular dynamics, and machine learning computational approaches to assist answer scientific questions collaboratively with experimentalists. She has scientific publications and has reviewed for international high impact journals.*

Enhancement of Syngas Production in Co-Pyro-Gasification of Biomass and Plastic Waste Materials: Computational Study

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The process of co-pyro-gasification of biomass and plastics appears to have the potential for increasing syngas production for power generation and thus minimizing the impact of plastic waste on the environment. This study was based on co-pyro-gasification of selected natural/synthetic polymers and cocoa pod husks as biomass material to ascertain the optimal ratios for enhanced volatile yields. Computational modeling also provided insights into the mechanisms of syngas production. The results showed that gasification of pure biomass commenced at 1500 K, whereas gasification of mixed plastics and biomass started at much lower temperature of 1000 K accompanied with higher syngas yield. Single and multiple plastics produced the most syngas while double plastics had detrimental impact on syngas production. For instance, single plastics with polyethylene terephthalate achieved 65 % increase in syngas yield. Mixed-plastics consisting of high-density polyethylene, low-density polyethylene, polypropylene, and polyethylene terephthalate, achieved an increase of 40 % - 55 % in syngas yield. Whereas antagonistic effects were observed in some double plastics systems such as polyethylene terephthalate and polypropylene. The results indicate that although plastics are instrumental in the thermodynamic equilibrium yields of syngas, the type of plastics and their groupings do also have a significant effect on the yields.

Keywords: Density functional theory; Molecular dynamics; Co-pyro-gasification; Reaction mechanisms; Kinetics; Thermodynamics.



I did my PhD in Physics. I am an expert of the Nanoscience, Nanotechnology, Materials and Fluids. I have skills in Experimentation, Numerical Simulation and Modeling. I have professional experience in porous materials, transport properties through nanoporous membranes, Interfacial and surface tension, wettability properties, polymers sciences, liquid crystals, liquid mixtures (water-oil, water-surfactant-oil ...), nanoconfinement, desalination and Water treatment, Filtration (MF, UF, NF), Reverse Osmosis-R.O and polymers and elastomers. I am owner of more than twenty publications and communications.

- ***2020- today:*** *Lecturer- Researcher- in Physics, Nanosciences, Nanotechnology and Materials*
  Department: *Advanced Sciences and Emerging Technologies (SATE)*
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  Laboratory: *LPQEN*
  University: *Cheikh Anta Diop of Dakar*
- ***Project:*** *Biomass and energy*
- ***2017- 2018:*** *R&D Engineer- Institute of Physics of Rennes- Rennes- France*
- ***Project:*** *Seawater treatment with Reverse Osmosis (R.O) membranes. Desalination, Filtration (Ultrafiltration- UF, Microfiltration- MF and Nanofiltration- NF).*
- ***2015- 2016:*** *R&D Engineer- Institute of Analytical Sciences and Physical Chemistry for the Environment and Materials (IPREM)-University of Pau and Pays de l'Adour (UPPA)-Pau France and MICHELIN-French tire manufacturer-Clermont- Ferrand*
- ***Project:*** *Modeling of Flow instabilities of nanocharged Elastomers and Polymers during extrusion process.*
- ***2014- 215:*** *R&D Engineer- Institute of Chemistry of Clermont- Ferrand, Clermont- Auvergne University- UCA (ex. Univ. Blaise Pascal)*
- ***Project:*** *Coarse- grained molecular dynamics simulation of liquid mixtures (oil- water, Water-Surfactant- Oil…) for applications in petroleum extraction, cosmetics, water treatment,*
- ***2010- 2013: PhD in Physics*** *(Nanoscience- Nanotechnology- Materials)*
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- ***ResearchGate: https://www.researchgate.net/profile/Makha_Ndao2***
- ***Google Scholar : https://scholar.google.com/citations?hl=fr&view_op=list_works&gmla=AJsN-F4YaZM387UflixZWA2r75Vd6ahuGLx43GvieaTv5JGlDEs0zsndMTnxWu44FCjCJEUGeQfbwskkblqIu5XoCQyd-VliQCTwfLXbhV5-oRjBwgUNUlQ&user=7ExGarYAAAAJ***
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Modeling Liquid- Liquid Mixtures Interfaces by Coarse- Grained Molecular Dynamics Martini- Force- Field

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We found liquid- liquid interface in several sectors of life. They have many applications in point of view of physico- chemistry, biology, and in oil extraction, cosmetics, pharmaceutical industry. However, their physico- chemical properties and the parameters influencing them remain poorly understood. The objective of this walk is to deduce and/ or predict these properties by Coarse- graining molecular dynamics simulation with Martini force- fields, by exploring mixtures liquid- liquid mixtures (binary and ternary) interfaces. Thus, I will first talk about the structural properties (volume density and interfacial tension) of these interfaces in binary mixtures: water- oil, water- alcohol, water- chloroform, … and their variation according to the shape, the chain length of the oil and the temperature of manipulation.
Finally, I will show you the influence of surfactant concentration on volume density and interfacial tension in ternary water- surfactant- oil mixture.

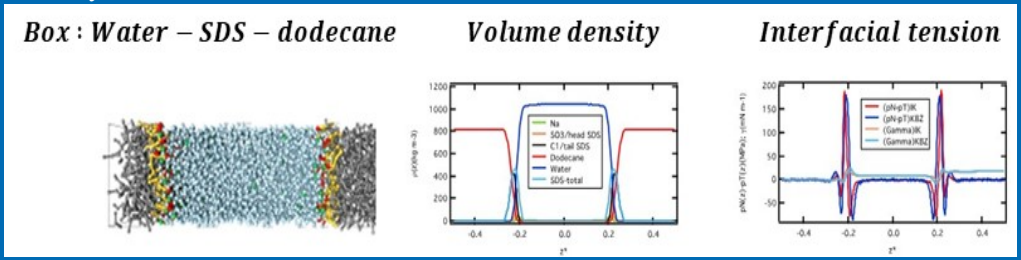


Figure: Ternary water- surfactant- oil mixture, volume density and interfacial tension

Keywords: Molecular dynamics simulation, coarse- grained, martini force field, volume density, interfacial tension, oil- water interface, surfactants at interface

Reference:

1. *Ndao et al., https://doi.org/10.1021/acs.jctc.5b00149.*
2. *Ndao et al., : https://doi.org/10.1007/s00214-016-2038-y.*



Graduated from the University Cheikh Anta Diop of Dakar, Cheikh Bop is currently a postdoctoral researcher at the Institut de Physique de Rennes (IPR). His work is focused on the excitation of interstellar molecules which is crucial to rigorously interpret observational spectra and derive molecular abundances, temperature and density of astrophysical environments such as star forming regions. Indeed, fully exploiting molecular observational spectra is a key step to better understand the chemistry that governs the enrichment of interstellar matter and therefore the origin of life on Earth.

As a member of the Pan-African School for Emerging Astronomers (PASEA) and the African Astronomical Society (AfAS), Cheikh is actively participating in astronomy outreach activities in Africa.

Non-LTE Modelling of the HCCNC and HNCCC Abundance in Astrophysical Environments

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The isomers of HCCCN, namely HCCNC and HNCCC, are widely observed in the interstellar medium and in circumstellar envelopes. Their abundance has been determined under the assumptionof local thermodynamic equilibrium (LTE) conditions or non-LTE ra-diative transfer models, but considering the collisional excitation of HCCCN as the same for all isomers. Chemical models for the prototypical cold cores, TMC-1 and L1544, reproduced the abundance of HCCCN fairly well, butthey tend to overestimate the abundances of HCCNC and HNCCC with respect to the observations. It is therefore worth revisiting the interpretation of the observational spectra of these isomers using arigorous non-LTE modelling. The abundance of HCCNC and HNCCC were then determined using non-LTE radiative transfer calculations based on the proper rate coefficients for the first time in thiswork. Modelling the brightness temperature of HCCNC and HNCCC when using their proper collision rate coefficients shows that models based on LTE or non-LTE with approximate collision data may lead to deviations of up to a factor of ∼1.5. Reinterpreting the observational spectra led us to significant differences relative to the observed abundances previously determined. Our findings suggest quite similar abundance ratios for the TMC-1 and L1544 cold cores as well as the L483 protostar. This work will encourage further modelling with more robust non-LTE radiative transfer calculations and future studies to revisit the chemistry of HCCCN and its isomers in cold molecular clouds.

Keywords: Molecular dynamic, cross sections, rate coefficients, molecular abundance, interstellar medium



Dr. Jean Paul Latyr Faye *is an expert in High Tc superconductors, Quantum Physics and Chemistry, quantum machine learning, and in the near-term quantum algorithms development. He contributed to elucidate the superconducting order parameter in graphene and in copper-based materials. Dr. Faye's work on investigating the superconductivity in graphene leads to the agreement that the symmetry of the order parameter is triplet and chiral. This work is published in Physical Review (Faye et al. Phys. Rev. B 92, 085121, (2015)) and has been cited by important experimental papers published in nature (Nature Communications 8: 14024 (2017)). Dr. Faye is also interested in Quantum computing where he develops quantum algorithms, adapted to current and near-term quantum hardware, should. Very recently, he contributes to the development of approximate quantum algorithms for addition and multiplication with applications to quantum neural network (Proceedings of the 19th ACM International Conference on Computing Frontiers, 2022).*

Chiral Triplet Superconductivity on the Graphene Lattice

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Motivated by the possibility of superconductivity in doped graphene sheets, we investigate superconducting order in the extended Hubbard model on the two-dimensional graphene lattice using the variational cluster approximation (VCA) and the cellular dynamical mean-field theory (CDMFT) with an exact diagonalization solver at zero temperature. The nearest-neighbor interaction is treated using a mean-field decoupling between clusters. We compare different pairing symmetries, singlet, and triplet, based on short-range pairing. VCA simulations show that the real (nonchiral), triplet p-wave symmetry is favored for small V, small onsite interaction U, or large doping, whereas the chiral combination $p+ip$ is favored for larger values of V , stronger onsite interaction U, or smaller doping. CDMFT simulations confirm the stability of the $p + ip$ solution, even at half-filling. Singlet superconductivity (extended s wave or d wave) is either absent or subdominant.



INVITED SPEAKERS

BZW-EF Ab-Initio Method Calculations of Ground State Electronic and Related Properties of Cubic Magnesium Silicide (Mg_2Si)

ALLÉ DIOUM,[1] YACOUBA I DIAKITÉ[2], YUIRY. MALOZOVSKY,[3] BLAISE AWOLA AYIRIZIA,[4] ABOUBAKER CHEDIKH BEYE,[1] AND DIOLA BAGAYOKO[3]

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New *ab-initio*, self-consistent method calculations to study electronic, transport, and bulk properties of cubic magnesium silicide (Mg_2Si) is presented. The local density approximation (LDA) potential to perform the computation regarding to Bagayoko, Zhao, and Williams (BZW) method, as improved by Ekuma and Franklin (BZW-EF). This BZW-EF method guarantees the attainment of the ground state as well as the avoidance of over-complete basis sets. The ground state electronic energies, total and partial densities of states, effective masses, and the bulk modulus are investigated. As per the calculated band structures, cubic Mg_2Si has an indirect band gap of 0.867 eV, from Γ to X, for the room temperature experimental lattice constant of 6.338 Å. The predicted band gap of 0.947 eV, from Γ to X, is obtained for the computationally determined equilibrium lattice constant of 6.206 Å. The bulk modulus of Mg_2Si of 58.58 GPa is in a good agreement with experimental value.

Keywords: Density Functional Theory (DFT), BZW-EF method, Band Gap, Density of States, Effective Masses, Bulk Modulus, LDA potentiel.

Computationally Driven Design of Earth-Abundant Materials for Renewable Energy Conversion and Storage

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The call for clean and sustainable energy sources has never been louder. Meeting the ever-increasing global energy demands, while at the same time drastically reducing carbon emissions from the over-reliance on and usage of fossil fuels remains one of the most critical challenges for humankind in the 21st century. Major breakthroughs in green energy technologies require advances in the fundamental science and engineering of novel materials. Achieving the required performance gains of energy materials, however, depends on exploiting the many degrees of freedom of materials development, including multiple chemical components, multilayer structures, nanoscale architectures, and tailored electronic structures. This introduces a huge complexity in the design process that must be understood and managed. With the rapid increase in computational power in the last decade, we are now at the threshold of a new era where predictive modeling and advanced simulations offer the most intelligent and efficient path forward to significantly expand the parameter space of materials development whilst lowering both costs and development times. In this talk, I will highlight the importance of employing atomistic simulations in synergy with novel experimental approaches to accelerate the rational design and synthesis of multiple earth-abundant material systems (e.g. perovskites, CZTS, FeS_2, Zn_3P_2, MoS_2, and WS_2) for different application types (photovoltaics, hydrogen evolution reaction, CO_2 conversion). The focus will be on understanding how surfaces and interfaces in photovoltaic devices and heterogeneous catalysts can be engineered to enhance their performance and stability. I will present the results of our recent studies on the beneficial role of iron sulfide pyrite–marcasite phase junctions for photo-electrochemical applications, where insights into energy band alignment and band offset estimation at semiconductor-semiconductor heterojunction will be unravelled. I will also shed some light on the role of lithium in enhancing the hydrogen evolution activity of MoS_2, where we demonstrate through a combination of theoretical modeling and spectroscopy methods with catalytic activity measurements that the enhanced hydrogen evolution reaction performance of Li_xMoS_2 is predominantly due to the catalytic promotion of edge sites by Li, which results in optimum Gibbs free energy of hydrogen adsorption (ΔG_H^*) at Mo edges than the S edges.

Keywords: Renewable energy; Photovoltaics; Thin films; Batteries; Atomistic simulations

Modeling Defects and Disorder in Polycrystalline Materials

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The functionality of the materials used for energy applications is critically determined by the physical properties of small active regions such as dopants, dislocations, interfaces, grain boundaries, etc. The capability to manipulate and utilize the inevitable disorder in materials, whether due to the finite-dimensional defects (such as vacancies, dopants, grain boundaries) or due to the complete atomic randomness (as in amorphous materials), can bring innovation in designing energy materials. With the increase in computational material science capabilities, it is now possible to understand the complexity present in materials due to various defects resulting in pathways required for optimizing their efficiencies. In this talk, I will provide a critical overview of such computational advancements specifically for designing realistic materials with various types of defects. I will discuss the traditional approaches (implemented via tools such as density functional theory, and molecular dynamics) as well as modern approaches such as machine learning that exist for understanding the impact of defects in polycrystalline materials, thereby identifying future opportunities for energy materials design and discovery.

Keywords: Computational Materials Modeling, Classical and Quantum Mechanics, Machine learning, Material Defects, Catalysis, fuel cells

Acknowledgments

The author acknowledges the Natural Sciences and Engineering Research Council of Canada (NSERC) Discovery grant program, Canada Research Chair (CRC) program, the Canada Foundation for Innovation (CFI) for infrastructure and operating funds. Computations were performed on the HPC supercomputer at the Calcul Québec (https://www.calculquebec.ca) and Compute Canada (www.computecanada.ca).

Theoretical Investigation of Magnetic Alloys

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Magnetic alloys are of technological importance in practical applications such as aerospace, automotive and data storage due their sufficiently high magnetic strength and resistance to demagnetization. Amongst them, FeCo is good magnetic material for actuator applications while Neodymium-based permanent magnets ($Nd_2Fe_{14}B$) are the potential for use in wind turbines and electric vehicles. In addition, MnPt alloy has received a great deal of attention in practical applications such as spintronics. However, there have been many new developments to improve their properties, as interest in magnetism and magnetic materials has grown dramatically. A multi-scale approaches were used to understand the structural, electronic, elastic and magnetic properties of these alloys. The stability of these alloys was determined from heats of formation, electronic density of states, phonon dispersion curves and elastic constants. Other interesting properties of magnetic alloys will be highlighted.

Keywords: Magnetic alloys, Density functional theory, Thermodynamic stability, Magnetic strength

Metamaterial for Microwave Application: Modeling and Design Using Babinet's Principle

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This work presents the modeling and design of negative permittivity metamaterial unit cells,based on complementary construction. The Babinet principle is used to design the unit cells. Rectangular and Circular Split Ring Resonator (RSRR CSRR) based metamaterials are presented.

For each of the structures, after obtaining the scattering parameters, the constitutivecharacteristics are extracted and discussed (Permittivity permeability, refractive index,dispersion diagram).

Applications to substrate integrated waveguide (SIW) filters are presented.

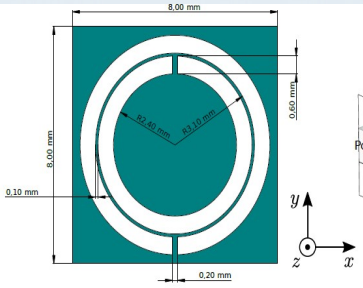


FIGURE 7.1 – Cellule Complémentaire du SRR (CoSRR)

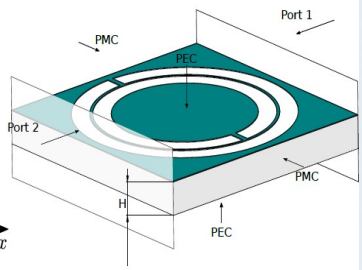


FIGURE 7.2 – Simulation CoSRR

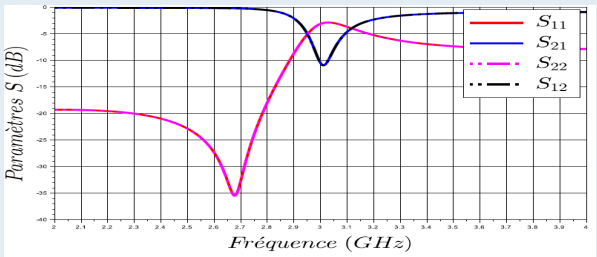


FIGURE 7.3 – Paramètres-S, Structure Complémentaire SRR

Keywords: Metamaterial, SRR, Babinet, SIW

Machine Learning in the Search for New Metallic Superconductors

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There is a need for ductile superconductors which can be drawn into wires and which have higher superconducting critical temperatures (T_c), higher than the ones for Nb-Ti alloys, for example, which are around 10 K. In the search for these superconductors, machine learning (ML) which is a subset of artificial intelligence (AI), can play an important role. We have used ML to search for superconductors which are metallic and, hence, very likely to be ductile/malleable. We developed two ML models – one using only the composition of materials and the other using both the composition and the crystal structures. These models are able to predict T_c for metallic materials with reasonable accuracy.

Keywords: Artificial Intelligence, Machine Learning, Superconductivity, BCS

Artificial Intelligence for Materials Science

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Artificial intelligence (AI) is transforming society, with tangible impact in fields ranging from computer vision, natural language processing, and recommender systems to robotics, biology, healthcare, and the physical sciences. In this talk, I'll discuss the many ways in which AI has been used to advance materials science. I'll highlight recent developments in using AI for discovering novel materials and evaluating their properties without relying on the traditional and costly density functional theory. I'll conclude the talk by discussing opportunities and challenges that lie ahead in AI-aided materials design.

DFT Study of Lithium and Oxygen Adsorption on Ruthenium Oxide (110) Surface

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Metal oxides are widely considered as excellent catalysts in lithium-air batteries to promote the production of stable discharge products and achieve superior electrochemical performance. The lithium–air (Li–air) battery is a metal–air electrochemical cell or battery chemistry that uses oxidation of lithium at the anode and reduction of oxygen at the cathode to induce a current. Despite various studies exploring the use of metal oxides as effective catalysis, the catalytic activity of ruthenium oxide (RuO_2) towards lithium and oxygen ions is not fully understood. In this work, we investigate the adsorptions of lithium and oxygen on the RuO_2 (110) surface using density functional theory (DFT) method. Due of the size of the supercell, and assuming that oxygen atoms occupy bulk-like positions around the surface metal atoms, only five values of (gamma) Γ are possible if constraint to a maximum of 1 monolayer (ML) of adatoms or vacancies: Γ= 0 surface is the stoichiometric surface, Γ= 1, 2 are the partially and totally oxidised surfaces, and Γ=-1, -2 are the partially and totally reduced surfaces. The addition of two oxygen atoms revealed the most stable adsorption energy is the mono-clear followed by bridging configuration. The lithium orientation between two bridging oxygen and in plane oxygen (bbi) orientation is much more stable, thus lithium generally prefers to adsorb where it will be triply coordinated to two bridging oxygen atoms and one in plane oxygen atom. Rutile RuO_2 has been widely considered as an excellent catalyst for the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) in non-aqueous.

Keyword: surface chemistry, ruthenium oxide, catalysis, density functional theory, adsorption energy



ORAL PRESENTATERS

Monolith $Cs_{1-x}Rb_xSnI_3$ Perovskite/Silicon Tandem Solar Cell Using SCAPS-1D Software

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This study focused on the simulation of photovoltaic characteristics of $Cs_{1-x}Rb_xSnI_3$ perovskite-silicon tandem solar cells using solar cell capacitance simulator (SCAPS-1D) software. The top cell was simulated independently with the structure ITO/$Cs_{0.8}Rb_{0.2}SnI_3$/PCBM/BCP/Al with an efficiency of 2.08 %. The effect of varying thickness, defect density, and doping concentration of the absorber layer, variation of PCBM Electron Transport Layer (ETL) thickness, doping concentration and CBO, and influences of the doped and undoped – ITO front contact of the tin-based perovskite solar cells were studied. Optimum open circuit voltage (0.9893 V), short circuit current density (30.04 mA/cm^2), fill factor (81.78 %) and efficiency (24.31 %) are determined. The bottom cell was simulated independently with reference to experimental data using the structure Al/c-Si (n)/c-Si (p)/c-Si (p+)/Au with an efficiency of 26.68 %. The monolithic $Cs_{0.8}Rb_{0.2}SnI_3$ perovskite – silicon tandem solar cell of the architecture ITO/$Cs_{0.8}Rb_{0.2}SnI_3$/c-Si (n)/c-Si (p)/c-Si (p+)/Au performance was analyzed by varying the thickness, doping concentration, and defect density of the active layers. Optimized parameters were as follows: top perovskite layer thickness (100 nm), doping concentrations (5 x 10^{19} cm^{-3}) and defect density (1 x 10^{13} cm^{-3}), and bottom silicon absorber layer thickness (50 µm), doping concentrations (5 x 10^{16} cm^{-3}), defect density (1 x 10^{12} cm^{-3}), with Cl doped – ITO (work function of 5.3 eV) as front contact of the tandem cell. Optimized outcomes of efficiency (29.82 %), open-circuit voltage (0.7992 V), short circuit current density (43.39 mA/cm^2), and fill factor (85.98 %) were realized for the 2T tandem solar cell.

Keywords: Tandem solar cells, Silicon, $Cs_{1-x}Rb_xSnI_3$ perovskite, SCAPS-1D

AB Initio Study of Structural, Electronic, Elastic, Mechanical, and Optical Properties of K_4XP_2 (X = Zn, Cd) Compounds for Optoelectronic Applications

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The structural electronic, elastic, mechanical and optical properties of the ternary compounds K4ZnP2 and K4CdP2 have been studied by means of density functional theory (DFT) using the plane waves method. The generalized gradient approximation with the Perdew-Burke-Ernzerhof (GGA-PBE) functional has been used as the exchange correlation. The study has shown that the compounds are thermodynamically and mechanically stable at zero pressure, making them suitable for synthesis and application for industrial use. In addition, the studied compounds have been found to be semiconducting with indirect band gaps of 1.068 eV and 0.947 eV for K4ZnP2 and K4CdP2, respectively. The refractive indices have been calculated to be 2.20 and 2.23 for K4ZnP2 and K4CdP2, respectively. The absorption coefficient of K4ZnP2 and K4CdP2 has been found to cover the UV-Vis regions of the electromagnetic spectrum; hence the compounds are good UV-Vis light absorbers and may therefore find potential in photovoltaic applications. The electronic states formation of valence band has been found to be due to contribution of P 3p and Zn 4p states in K4ZnP2, while in K4CdP2 is due to P 3p and Cd 5p, on the other hand the conduction band is due to contribution of the unoccupied Zn 4p and Cd 5p states in both compounds, respectively.

Keywords: DFT; Bandgap; Mechanical properties; Optical properties; Photovoltaic applications

SCAPS 3201 Simulation of Tunable Heterostructured P-CdTe and N-CdS Thin Films-Based Solar Cells at Varied Growth Cathodic Potential.

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The paper presents the utilization of numerical simulation, SCAPS 3201, and an electrometer in the investigation of electrical behaviour at the interface of the heterostructured Cadmium telluride and cadmium sulfide thin films. Indeed, there is a noticeable drastic improvement in the performance of electrodeposited p-CdTe and n-CdS thin film-based solar cells, tuning the growth potential. All the parameters such as electrical conductivity types and energy band gaps used in the simulation were obtained from the various analytical procedure employed as against the conventional mode of application of the SCAPS simulation. In most research works on CdTe/CdS-based solar cells, the conductivity type, p-type, and n-type used in SCAPS simulation are based on assumption. However, in the study, the material's conductivity type employing photoelectrochemical (PEC) cell measurement helped in the identification of p-type CdTe and n-type CdS. The material's properties were examined using X-ray Diffractometer (XRD), scanning electron microscopy (SEM), ultraviolet-visible spectrophotometer (UV-VIS), (PEC), and electrometer. The energy band gaps at varied cathodic potentials and the grain size of CdTe thin films were estimated as 1.47-1.89 eV and 56 nm while that of CdS were 2.37-2.46 eV and 115 nm. The extracted electrical parameters (J_{SC}=15.22, V_{oc}= 749, FF= 0.82 and QE= 9.0% at 520 nm) using SCAPS and electrometer are evidence of the improvement made and the results from both the SCAPS and electrometer are in tandem.

Keywords: CdTe/CdS thin films; electrodeposition technique; heterostructured based photovoltaic; electrical conductivity type; SCAPS.

First-Principles Study of $Ti_{50}Ru_{50-x}y_x$ (Y= Ni, Pd, Pt) With Prospect to Induce SME on Stable Cscl-Type $Ti_{50}Ru_{50}$ Phase

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The equiatomic (near 50:50 compositional range) of TiRu belongs to the CsCl-type intermetallic compounds that are derivatives of Group 4 (Ti, Zr and Hf) together with Group 10 metals of the periodic table of elements. The CsCl-type intermetallics has shape memory effect (SME), a phenomena that occurs on certain class of materials with an ability to undergo phase transition during crystallization. This advanced functional materials' property of CsCl compounds is enabled by martensitic phase transition from an ordered B2 phase of high symmetry at high temperature to phases of lower symmetries such as $L1_0$, B19 or B19' upon cooling to lower temperatures. Peculiarly so, $Ti_{50}Ru_{50}$ with similar ordered B2 at high temperature remains ordered and stable with no phase transition down to room temperatures. In this study the first-principles calculation based on density functional theory (DFT) is used to investigate the structural, thermodynamic and electronic properties of the stable $Ti_{50}Ru_{50}$ compound by systematically substituting part of the Ru atoms with ductile group 10 metal (Ni, Pt and Pt) atoms. This will be conducted with an aim to unstabilize B2 $Ti_{50}Ru_{50-x}Y_x$ ternary phase at 0K, and promoting martensitic phase transformation that could yield SME.

Keywords: Density functional theory (DFT), Elastic constants, Phase stability, Shape memory effect

A Computational Study of the Thermodynamic and Magnetic Properties of Co-Alloyed Mnpt

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Magnetic functional materials remain an area of research interest for applications in electronic devices. Among these materials, MnPt alloy has received a great deal of attention in practical potential applications such as spintronics due to its high thermal and magnetic stability. It was reported previously that $L1_0$ MnPt alloy shows ferromagnetic ordering at room temperature. In this study, the effect of partial substitution of Pt with Co on thermodynamic and magnetic properties is being investigated using density functional theory. The thermodynamic, magnetic and mechanical properties were determined to check the stability of $Mn_{50}Pt_{50-x}Co_x$ alloys (x=6.25, 12.5, 18.75, 25) alloys. The calculated lattice constants of $Mn_{50}Pt_{50}$ agree well with available experimental results. It was found that $L1_0$ $Mn_{50}Pt_{50-x}Co_x$ are thermodynamically stable due to the negative heats of formation. In addition, the results showed that the $L1_0$ phase has the lowest heats of formation when the c/a ratio is 1.10 for 6.25 at. % Co. Based on calculations, $Mn_{50}Pt_{50-x}Co_x$ can achieve a ferromagnetic state by varying the tetragonality ratio from 1.10 to 1.30. Overall magnetic moments improve with an increase in Co compositions when the c/a ratio is 1.10. Furthermore, the ductility of $Mn_{50}Pt_{50-x}Co_x$ is predicted using Pugh and Poisson's ratio. The obtained results reveal that $Mn_{50}Pt_{50-x}Co_x$ alloys exhibit attractive magnetic and mechanical properties for future magnets in spintronics applications.

Keywords: MnPt, Density functional theory, Stability, Magnetic strength

Magnetic and Mechanical Properties in Pd-Doped B2 Feco Soft Magnetic Materials

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FeCo alloy plays an important role in soft magnetic materials with a wide range of technological applications due to its high saturation magnetization and Curie temperature. However, this alloy displays low levels ductility at room temperature. The ductility of this alloy can be improved by the ternary addition of Pd. In the current paper, a density functional theory supercell approach was used to generate B2 $Fe_{50}Co_{50-x}Pd_x$ structures and different properties were evaluated at different atomic compositions to determine their ductility at room temperature. The structures were fully optimized to obtain better equilibrium ground-state properties for both binary and ternary systems. The stability of $Fe_{50}Co_{50-x}Pd_x$ was evaluated from the heats of formation, elastic properties, magnetic properties, and phonon dispersion curves. The DFT results of FeCo gave equilibrium lattice parameter and heats of formation in good agreement with the experimental findings to within 1%. It was found that the $Fe_{50}Co_{43.75}Pd_{6.25}$ structure is thermodynamically stable due to the negative heats of formation. The calculated Pugh and Poisson's ratio confirm that alloying with 6.25 at. % Pd effectively improves the ductility. It was also found that $Fe_{50}Co_{43.75}Pd_{6.25}$ showed positive shear modulus, a condition of stability in agreement with phonon dispersion curves. Furthermore, the ternary addition of Pd to the FeCo system resulted in enhanced magnetic properties. These findings reveal that B2 Fe-Co-Pd alloys can be used as magnetic components and actuators for the automotive industry operating at high pressures.

Keywords: FeCo alloys, Mechanical properties, Phonons, Ductility

Thermoelectric Modelling of Hybrid Based-Perovskite Organic-Inorganic and Bulk-Heterojunction Organic Photovoltaic Devices

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Thin films of Methylammonium lead iodide ($CH_3NH_3PbI_3$) perovskite and blending of poly (3-hexylthiophene-2, 5-diyl) and [6, 6]-phenyl C61-butyric acid methyl ester (P3HT: PCBM) are deposited on substrates under open-air conditions and high relative humidity for realizing hybrid organic-inorganic based perovskite and Bulk-Heterojunction Organic Solar Cell (BHJ-OSC) solar cells. Under AM 1.5 g illumination, devices have been characterized by measuring the current–voltage I(V) characteristics. New theoretical model has been developed to give insight the thermo-electrical properties such as the free charge distribution generated within the bulk of the active layers under bias. Then, the dependence of the charge carrier recombination at the active's layer/electrode interfaces on the charge carrier density and the photocurrent density are evidenced. Moreover, our model allows evidencing the energy losses at the electrodes contact.

Keywords: Characterization - Modeling - hybrid solar cell - Perovskite – Blend - planar heterojunction

A Molecular Dynamics and Mesoscopic Dynamics Simulation Study on the Miscibility of Polyglycolide with Various Polymers

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Molecular dynamics simulations using the Forcite, Blends Modules and Mesodyn are used to study the miscibility of mixtures between polyglycolide with the polystyrene, polyacrylonitrile, polylactide and polyethylene. For the evaluation of the energy, the simulations of the binary mixture are achieved in the framework of the Flory – Huggins Model. Seven polyglycolide (PGA)/polyethylene (PE) blends (with weight ratios of 80/20, 70/30, 20/80, 30/70 and 50/50), as well as pure PGA and PE, are evaluated. The free energy of mixing, the Flory – Huggins interaction parameter, phase diagrams, order parameters, and radial distribution function are analyzed. The results show that when the Flory – Huggins interaction parameter Chi is close to 1, the polyglycolide is miscible with all polymers at a temperature above 378K. The PGA/PE blends have good miscibility for all the weight ratios investigated. The phase diagrams of all the binary mixtures are present one critical point. The miscibility of mixtures at that critical point corresponds to an optimal mole fraction of 0.5. This is further supported by the morphologies of PGA/PE blends. The phase separation kinetics of PGA/PE blends is then examined using density profiles calculated from the Mesodyn approach to examine the mesoscopic morphology of the blends. Our results are in agreement with those found in the literature.

Keywords: Polymers, Polyglycolide, Miscibility, Molecular Dynamics, Blends

Theoretical study of chemical reactivity descriptors of some proposed drugs for COVID-19

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Nanotechnology has been used in medicine as a new tool for novel diagnostics, medical imaging, site-specific, and target-oriented drug delivery. Drug delivery is a promising, multi- field research area with several potential opportunities. Computational studies can be implemented to predict molecular interactions between pharmaceuticals and nanoparticles to build next-generation drug carriers.
This study focuses on computational studies of chemical reactivity descriptors of someproposed drugs for COVID-19. Density functional theory calculations were used to optimize the structure and investigate the frontier orbitals and the chemical reactivity descriptors of these drugs. The frontier orbitals, which include both the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), play an essential role in molecular interactions and chemical reactivity of molecule. Polarizability, which determines the response of the susceptibility of a molecule to an approaching charge, is higher in the morecomplex drugs such as Hydroxychloroquine, Remdesivir, and Ivermectin compare to the smaller drugs. The HOMO and LUMO orbital energies were calculated to obtain the energy gap of the studied drugs, which is in the following order: Favipiravir < Hydroxychloroquine, Remdesivir < Ivermectin < Artesunate < Artemether < Artemisinin. Generally, molecules witha larger energy gap have lower chemical reactivity and higher kinetic stability.

Keyword: Nanomedicine, Chemical reactivity descriptors, Computational Chemistry, Density Functional Theory, Frontier Orbitals

Effect of Silver Nanoparticle Size on Interaction with Artemisinin Drug: First Principle Study

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According to their antiviral and antibacterial capabilities, silver nanoparticles hold great promise in a wide variety of applications, including drug delivery carriers. The coating properties of silver nanoparticles (various sizes ranging from 1 to 5 nm) with the most commonly used anti-malarial drug, artemisinin, were investigated in this study using quantum mechanical and classical atomistic molecular dynamics simulations in order to determine their suitability for use as drug delivery in the treatment of malaria and COVID-19 diseases. Density functional theory (DFT) at the B3LYP/6-311++g(d,p) level of theory was used to simulate the optimal structure, frequency, charge distribution, and electrostatic potential maps of artemisinin. The adsorption of drugs on the Ag nanoparticle (55 silver atoms) was investigated using DFT simulations. Then, using molecular dynamics simulations, the coating of AgNPs (various sizes) with drug molecules was investigated. The influence of AgNPs' size and composition on the coating with artemisinin was determined in order to identify the most suitable candidate for drug delivery. This type of modeling may aid experimental groups in developing effective and safe therapies.

Combining Multimodal Data of Fatigue Fracture Surfaces for Analysis in a CNN

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Images of fracture surfaces are rich in information and have long been examined to determine fracture characteristics such as initiation site and crack growth mode. Computer vision and machine learning techniques, including convolutional neural networks (CNNs), are new methods that can be applied to microstructural images to make predictions and connections between the microstructure and material responses. For fatigue failure, a goal is to connect the visual appearance of the fatigue fracture surface to fatigue characteristics such as loading values, crack length, and crack growth rate. This allows quantitative information to be attained from fracture surfaces where specific loading conditions are unknown. Scanning electron microscopy (SEM) has been the primary image modality for studying fracture, but surface height information acquired from Scanning White Light Interferometry (SWLI) and compositional contrast from Backscattered electron (BSE) can provide additional useful information.
This project collects multimodal data from Ti-6Al-4V fracture surfaces in the form of BSE and SEM images and SWLI height data and combines them to train a CNN to identify high stress points, crack initiation sites, and predict values such as loading ratio and crack growth rate. Through data fusion, these image modalities can be combined to improve the recognition of subtle features on the fatigue fracture surface. Using standard computer vision techniques to register the images and transfer learning to construct the CNNs the stated quantitative values can be predicted. The images used to develop this model, image registration technique, creation of the CNNs, identified fatigue properties, and fracture characteristics will be presented.

Keyword: Computer Vision, Fatigue, Fractography, Ti64, Machine Learning

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Defects Studies in Thin Films of MAPbBr3 Perovskite: A DFT Based Study

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Metal halide perovskites have potential industrial application in photovoltaic modules. Despite the high efficiencies reported in this type of materials, charge carrier mechanism remains a subject of discussion. This study is investigating the types and impact of defects in Methylammonia Lead Bromide (MAPbBr3) using the Density Functional Theory (DFT) approach. Dopants such as bismuth shall be added to MAPbBr3 and evaluated on their optoelectric properties and defects. DFT calculations will be employed in Quantum Espresso code.

Keywords: metal halide, DFT, CH3NH3PbBr3, defects.

The Continuous and Impulsive Grazing Model in a Sahelian Region

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Sahelian pastoral livestock farming plays a major role in the economies of West African countries. With a great diversity of high species, it contributes to the food and nutritional security of rural and urban households. Nowadays, in addition to the effect of climate events, speculation, price volatility and the substitution effects of imported products by local products, exacerbate the volatility of the terms of trade. So at this level, the pastor can harvest in the herd population for survival reasons. Hence, in this paper, we aim to build and analyze a mathematical model for resource-livestock herd interactions in a Sahelian region by first taking into account a continuous harvest for various needs. Since several months or even years can pass between two harvests, a more realistic way is to consider that this harvest is done impulsively because it intervenes very often at precise moments for known reasons (sale, bequest, slaughter, etc.) [1; 2]. We performed a qualitative analysis of our model and numerical simulations are provided in order to illustrate our theoretical results and to support the discussion.

Keywords: Pastoralism, Grazing, Continuous, Impulsive, Sahalian Region.

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Corrosion Cracking Prediction Models

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Corrosion Cracking (CC) is a form of environmental cracking which leads to structural damage and progressively to catastrophic failure, if not checked on time. When engineering structures are in operation, huge amount of money is spent to either lessen or control the damage caused by CC. The likelihood of failure resulting from CC can be predicted using empirical models that consider the contribution of the environment and other factor such as stress ratio. This paper discusses the influence of the environment on the crack growth rate in steels during corrosion cracking at the crack-tip and the effects of applied stress when exposed to corrosive environments.

Keywords: steels, corrosion cracking, fatigue crack, paris regime, stress intensity factor range

Adsorption of Br_2 Molecule on the Fe/W(110) Substrate: Energetics, Electronic and Magnetic Properties

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Using spin-polarized density-functional calculations with generalized gradient approximation (GGA) as the exchange-correlation functional, we report the energetics of adsorption, as well as the electronic and magnetic properties of homonuclear brominemolecule deposited on the Fe/W(110) substrate. The Fe/W(110) substrate consist in Fe monolayer on the topmost W(110) layer such that the Fe atoms are bonded on the bridge adsorption sites of the W(110) surface. Our calculations show that when the Br2 moleculeis adsorbed in parallel, oblique or vertical orientation with respect to the surface, the molecule dissociates. However, when the Br2 molecular adsorption is perpendicular to the bridge or top sites, non-dissociative adsorption occurs. We also found that the observed Br2 adsorption properties depend on the interaction between the 4p orbitals of adsorbed bromine specie and the Fe-3d orbitals of Fe atoms of the Fe/W(110) substrate. Furthermore, it is shown that when the bromine atoms are attached on its energetically preferred adsorption sites, the magnetic moments of Fe atoms are reduced while magnetic moment is induced on the bromine atoms. These results are consistent with a previous work on the O2 adsorption.

Keywords: Spin-polarized calculations; Bromine; Iron/tungsten substrate; Adsorption properties; Electronic structure; Magnetic moments.

Molecular Dynamics Study of the Influence of Temperature and Pressure on egg White Lysozyme.

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The effects of temperature and pressure are important and essential for a complete understanding of living organisms because their ability to survive under such conditions is linked to the structural stability of their proteins. Therefore, stability appears as a fundamental property to the understanding of the structure and function of these proteins. Among these various proteins, lysozyme, a protein involved in the defense against bacterial infections and found in many animal species (tears, saliva, sweat, nasal secretion as well as in egg white), has been the subject of numerous studies. The model lysozyme of our study is that of hen egg white, due to its relatively simple structure, its high interracial reactivity and its remarkable physicochemical properties, it has been widely used in recent years in multiple applications such as the food and pharmaceutical industries as well as in biotechnology. It is in this context that we study the influence of two physical parameters, namely temperature and pressure, on the conformational stability and dynamics of hen egg white lysozyme. To do so, we applied molecular dynamics simulation techniques, implemented in the GROMACS code, in order to understand how temperature and pressure affect the native conformation of this protein, in other words its activity. We performed simulations at different temperatures (300K, 340K and 400K) and pressures (1bar, 1000bar and 3000bar) by measuring the root mean square deviation (RMSD) and the radius of gyration (Rg) to evaluate the stability and compactness of our protein respectively. The root mean square deviation and radius of gyration showed considerable variation with increasing temperature while a small variation was found with increasing pressure. Thus lysozyme rapidly loses its conformational stability under high temperature conditions while high pressure has a very small effect on its conformation. This study is of practical interest as these two parameters are used for sterilization and bioconservation of products in the food and pharmaceutical industries.

INSIGHT DESCRIPTION OF THE PHOTO-INDUCED ELECTRON TRANSFER (PET) IN LIGHT-HARVESTING SYSTEMS PROCESSES

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This study aims to provide insight on the light-driven charge transport processes in the scope of solar energy conversion and dye-sensitized solar cells based on a fully theoretical approach. The project will employ and develop theoretical and computational methods to assess photoinduced electron transfer (ET) processes in integrated n-type/p-type semiconductors (n-SC/p-SC) and guide the design of novel photosensitizers (PSs) with desired properties and functions. The computational studies at the SC-PS interface are conducted applying state-of-the-art quantum chemical calculations, such as density functional theory (DFT) and time-dependent density functional theory (TDDFT) in combination with ab initio molecular dynamics (AIMD) addressing the light-driven charge transport cascades among the PS and the n/p-SC as well as between the PS and the redox shuttle (RS). The computational evaluation and tuning of the photo-induced electron transfer (PET) processes is of outstanding importance in the field of solar energy conversion. In order to computationally assess the PET kinetics at the n/p-SC-PS-RS interface, we will extend our currently applied approaches, which are based on semiclassical Marcus theory and quantum dynamical simulations.

Keywords: Theoretical chemistry; p-type and n-type semiconductor; dye-sensitized solar cells; electron transfer theory; TDDFT; molecular dynamics



POSTER **PRESENTERS**

Modelling and Simulation of the Hot Plate Method with Passive Guard: Sensitivity Study of the Model to Thermo-Physical Parameters

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In the context of the objective of reducing the energy consumption of buildings, a lot of research is currently being carried out in order to develop building materials, and in particular more efficient insulating materials whose production has little impact on the environment. The use of insulating materials makes it possible to attenuate the transfer of heat through the walls of the building. Thus, the determination of the thermo-physical properties of these materials is necessary. The characterization of materials with large dimensions is almost impossible or excessively expensive for the laboratory. Therefore, the implementation of measurement methods that can characterize samples of size 10cmx10cm, is necessary. In this study we have performed a modeling of the hot plate method with passive guard in unsteady regime. After modeling the system, we performed a simulation with the COMSOL Multiphysics software. The results obtained with Comsol are considered as a numerical experiment. The complexity of these differential equations does not allow us to use all the analytical methods effectively and efficiently. One of the solutions is to adopt a numerical approach for the resolution. A MATLAB program allowing to determine the temperature evolution along the material is developed. The developed model allows us to make a study of reduced sensitivities on the thermo-physical parameters of our material.

Keywords: Materials, reduced sensitivities, estimates, thermal diffusivity, thermal conductivity

Mesostructured Hybrid Based-Perovskite Solar Cell Optical and Electrical Modeling: Influence of the Incident Light Wavelength

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Abstract: Analytical model is developed to give insight into the influence of the incident wavelength of the incoming light illumination on optical and electrical properties mesostructured hybrid perovskite-based solar cell for different photoactive layer thickness. Bruggeman theory and T-matrix are used to compute the analytical expressions of optical parameters such as absorption coefficient and generation rate. Then, the short-circuit current density is deduced from the continuity equation. The absorption coefficient of the photoactive layer decreases with high incident wavelength of the incoming light of the visible spectrum (400-800 nm) while the absorbance and generation rate grow up with the phototactive layer thickness. The current density increases with illuminated wavelength ranging 400-520 nm while it decreases with higher active medium (TiO2 +Perovskite) layer thickness ranging from 500 nm to 1.7 µm. Beyond to 520 nm of the wavelength of the incoming light, the current density decreases to vanish at 800 nm. As finding in the literature, it can be noticed high absorption, charge carriers generation and current density for low wavelength in the visible spectrum which correspond to high energies.

Keywords: *Modelling, Hybrid solar cell, perovskite, Mesostructure, Bruggeman theory, T-matrix*

Insight into Stability of Natural Plant of Betalaine Anthocyanins as Pigments for PV Systems

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Various dyes are used as color indicators in carotenoids and curcumin regarding their pH in solution. Indeed, red betanidine and anthocyanins in acidic medium, turns into blue when the pH is up to three (3). Density functional theory (DFT) calculations is performed potential of natural sources of betalain (the opuntia ficus indica) and anthocyanin (hibiscus sabdarifa L.) as natural dye in application in DSSC for performing dye sensitized solar cell (DSSC) instead of synthetic and artificial one. Basically, calculations of various deprotonations cases related to the dye acidic pH for energies level alignment with the semiconductor (TiO_2) and electrolyte I_3^-/I^- systems. In addition, electronic spectra of the various molecules dye are investigated using Time-Dependent Density Functional Theory calculations. These present results give insight into prediction of conditions improvement of DSSC performance.

Keywords: Density Functional Theory – Theoretical characterization – Natural Plant – DSSC – Deprotonation - hibiscus sabdarifa L.

DFT Calculations of Chemical Constituents of Anthocleista Liebrecthsiana for PV Applications

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Anthocleista liebrecthsiana is a traditional and medicinal plant piece use for bacterial infection treatment. However, it contains a wide variety of molecules which alternately deserves to be tested for new application fields such as photovoltaics and electrochromic materials. Theoretical model based on density functional theory (DFT) calculations is used for geometry improvement of molecules. Molecular structure of compounds are determined from proton, carbon NMR chemical shift. Then, absorption wavelength analysis has been performed using DFT/B3LYP method with a 6-311+G(d,p) basis set. Time-Dependent Density Functional Theory calculations give into insight the electronic spectra to learn more about the matching of theoretical and experimental results of light harvesting. Moreover, in order to characterize electron distribution excited states and study orbitals configuration population are considered. Various component are classified regarding to new application field in the scope of energy.

Keywords: Density Functional Theory – Theoretical characterization – Natural Plant – DSSC - Anthocleista liebrecthsiana

Study of the Stability of Aluminene by Density Functional Theory (DFT) Method

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In this paper we study of the stability of aluminene, a two-dimensional monolayer aluminum structure. With (DFT), we use density functional theory to study the stability of aluminene under these different configurations: hexagonal (graphene), buckled (silicene), Trigonal (space group p3ml) and orthorhombic (space group pmmn). We were able to find through our study that only the graphene-type and silicene-type structures were stable. The study of their electronic structure has shown that both graphene-type and silicene-type structures have a metallic behavior. Compression and stretching of the stable structures revealed that the graphene-type configuration is stable up to 10% compression and 29% stretching. The silicene configuration starts to become unstable from 3% (stretching) however it remains stable up to 15% compression.

Keywords: DFT, aluminene, stability, band structure

Simulations of Antireflecting Coating on a Monocrystalline Silicon Solar Cell: Influence of Optical Parameters on a Double Layer.

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The decrease in the reflection of light on the lens is due to the porosity of the surface on a very thin thickness due to the refractive index became lower at 30 %. It is well known that the deposition of one or more layers of certain materials on the front face of the photovoltaic cells and optoelectronic devices such as lasers, diodes, reduces the reflection of the incident light, which improves the performance of the cells. Solar energy, whose efficiency varies around 60 %. In this study, the influence of the thickness of an antireflection layer, in this case SiO_2, TiO_2, MgF_2, Si_3N_4, ZrO_2 on the spectral response of the solar cell to silicon which passes up to about 90 % for a layer of $MgF_2/TiO_2/Si$ whose refractive index values are respectively n = 1.3767 and n = 2.5742 quite far apart.

Keywords: solar cell, antireflection coating, spectral response, thickness, refractive index.

Prediction of Atmospheric Turbulence by Means of WRF Model for Astronomical Observations

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A major obstacle for ground-based observations is the micro-fluctuations of temperature in the atmosphere which, modifying the refractive index of the air, randomly scramble the propagation of optical waves and cause a loss of information. The choice of a site for a future observatory is crucial for the long-term development of national astronomy. Thus, the image quality or seeing has become one of the criteria retained in the final decision making for the choice of sites. The prediction of atmospheric and turbulence conditions is of great interest for the astronomical community. However the use of a numerical approach becomes crucial for the characterization of atmospheric and optical turbulence conditions.
In this study, a numerical approach based on the Weather Research and Forecasting (WRF) of meteorological parameters (temperature, relative humidity, wind speed and direction) as well as the optical turbulence conditions (C_n^2) of the forecast model for all three target sites in Senegal. We also present the seeing obtained for each site and other integrated parameters of the vertical profiles of atmospheric turbulence.

Keywords: Atmospheric turbulence, Seeing, Weather Research and Forecasting

Numerical Approach to Pattern Formation in Anisotropic Diffusion Reaction Models with Fractional Caputo Operator

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This paper deals with the analysis of Turing instability conditions in a resourceherbivore model with anisotropic harvesting and diffusion using a fractional derivative operator in the Caputo sense in time. After an analysis of the stability of the model equilibria, we perform an analysis of the Turing instability theory taking into account the fractional derivative in time. For the numerical analysis of the model, we discretise according to each independent variable (time, space). The discretisation in time of the model equations is done by a L1 scheme based on a finite difference scheme for the fractional operator and for the diffusion operator an implicit scheme is used. For the discretisation in space, a five-point finite difference scheme is used for the diffusion operator. Finally, based on these numerical schemes, we provide some numerical simulations to illustrate our qualitative results and to support the discussions.
Keywords. Turing instability. Fractional caputo operator. Reaction-diffusion systems.



SYMPOSIUM-08
MATERIALS EDUCATION AND **NETWORKING**



KEYNOTE SPEAKERS



***Dr. Surya Raghu**'s expertise is in research commercialization - transitioning of ideas, inventions and innovations into commercial products. He obtained his Ph.D. in mechanical engineering from Yale University and is the founder-president of a high-tech company - Advanced Fluidics, LLC since 2001 and founding partner ET Cube International, Inc. since 2013. He is also currently a visiting professor at Wits University, S. Africa. His earlier affiliations were with Yale University, Technical University of Berlin, SUNY Stony Brook and Bowles Fluidics Corporation. Dr Raghu has inventions related to aerospace, automotive, consumer and bio-technology applications and has been awarded 15 US patents. He has been a co-director and/or invited speaker of more than 40 workshops in about 25 countries on Entrepreneurship, Research Commercialization, Knowledge/Technology Transfer for Scientists, Engineers, University faculty, technology transfer officials and IP policy committees.*

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Upskilling Students and Researchers for Innovation and Entrepreneurship

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There is an urgent need to instill skills of innovation in the students (the future scientists and engineers) who can apply their research and scientific knowledge to address societal and/or market demands that need scientific and technological solutions. Ability to translate, transform or extend knowledge from one field or application to another are critical in such endeavors. This might also have an upstream effect on the type of research projects chosen by the students and faculty. Entrepreneurial skills imparted to them may also provide a pathway for commercialization of the creative outputs of both faculty and students through start-ups created for this purpose, thus transforming themselves from employment seekers to employment creators. Such additions to the curricula and their outcomes could enhance the University's role in the regional economic and social development. In this presentation, I will discuss the need for integrating formal training in these concepts of innovation and entrepreneurship into university education programs.



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Mouhamadou Mansour Faye was born in 1963 in Dakar. Pr Faye holds a Master's degree in Applied Physical Sciences from Cheikh Anta Diop University in Dakar, then a diploma of advanced studies in 1989 and a Doctoral thesis in Solid State Physics from Paul Sabatier University., Toulouse, France, in 1992. Since 1992, he has been teaching Physics in the Department of Physics at Cheikh Anta Diop University in Dakar. On the scientific level, Pr Faye has worked on modelling, simulation and observation with transmission electron microscopy in the field of ion implantation in semiconductors and then in nonlinear physics. In terms of e-Learning and pedagogy, Pr Faye holds since 2007 an International Masters in e-Learning at the Kurt Bosh University Institute, Switzerland. He is at the origin of various initiatives aimed at introducing ICT in education and training and brought his expertise to several national and international projects and institutions. Pr Faye was the first Coordinator of the Virtual University of Senegal from 2014 to 2016.

Education and Training in the Face of Ongoing Challenges and Changes: The Case of Senegal

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The implementation of adequate policies has enabled the number of the world's children to have access to basic education. This has had many positive results especially in terms of equity and fairness in access. However, the main consequence is the significant increase in the number of learners at higher levels of the education system. It was therefore necessary to build new colleges and universities, to train and recruit new teachers, to release the adequate means in order to take charge of the new needs. However, that is commonly observed, is that the response is often below the real needs. This has led to an accumulation of tensions at the level of the reception capacities of the training structures, to the insufficient number of the teaching staff, to the lack of skills for a great number of these teachers, to a growing dissatisfaction with the strategies of training adopted and often to a questioning of the adequacy of the products formed in relation to the needs of society. On the other hand, our world is facing profound changes since several decades at a pace and scale never equaled. These changes are mainly driven by the development of science, technology and an unprecedented telecommunications ecosystem. This certainly raises the place of science, technology and the new communication environment in our training systems. Senegal, like many countries in the world, especially in Africa, experiences, initiates and sometimes undergoes these changes.

The purpose of this communication is to take a retrospective look at the road traveled and to share the lessons learned.



Dr. Mahamadou Lamine Sagna

Currently Professor of Sociology at WPI (Worcester Polytechnic Institute), Dr. Mahamadou Lamine Sagna holds a Ph.D. in sociology and Master Degree in Business Administration and Ethnic-psychiatry in France. His multidisciplinary background provides a thoroughness and fluidity as he addresses complex intersections between sciences, economics, gender, culture, and power—specifically in how they relate to poverty, his personal field of interest. His interdisciplinary approach frequently enriched his pedagogy.

Prior to WPI, Dr. Sagna taught at American University of Nigeria, Schiller University in Paris, Princeton University and was a Visiting Professor at the University of Maryland. He has participated and organized many multidisciplinary seminars, symposia and he has written several articles and a book Money and Society, and on Politics, Violence, Racism and Religions in America- Cornel West Matters.

In addition, amount of time and passion Dr. Sagna dedicates to community. He is member of many professional networks, and he is a founder and executive director of "Re-Source/Sununet" a Senegalese Diaspora organization (which is represented by chapters in Africa, America, Europe, Asia).

Dr Sagna speaks four languages fluently (French, English, Mandingo, Wollof) and is competent in "Creole" Portuguese and Spanish.

STEM Education in Africa: Reflection on Some Conditions of Possibilities

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The impact of technology on people's lives is enormous, and the learning and dissemination of scientific results are paramount in our contemporary world. On this note, our paper focus on the numbering systems of African populations and how to develop a STEM-education system in Africa – a proposition that will help understand the symbolic systems of the populations. Indeed, the value of science or technology lies in its degree of use, which reveals the systems of truth representation. Science as a site of truth challenges the other sites of truth such as, Art, Love, and the Collective



INVITED SPEAKERS

Concurrent Approach to Research Leading to an Immediately Practical Applicability of Material Science and Engineering

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This work describes how a concurrent and multi-disciplinary approach to education in material science and engineering can lead to immediately practical and applicable student research outputs. This work adapts the concurrent engineering approach used to design spacecrafts and space missions to the design of student research projects.

Piloted at the Nelson Mandela University, the approach requires a central project around which every faculty involved would work. The proposed project is the design of a space mission. This is because space missions by their very nature impose a level of rigor and quality standards that are immediately applicable in real-world situations. Space missions are inherently multi-disciplinary and multi-cultural. To be successful, it requires people from different backgrounds and cultures, and with different disciplines (engineering and non-engineering) to successfully work together. Space missions also pose various levels of challenges. This means that a single mission could simultaneously generate multiple bachelors, masters, and doctorate level projects in many different disciplines. Research projects are defined as follows:
From mechanical engineering, students to do mechanical design. From electrical engineering students to do harnessing, communications, and power systems design. From mechatronics, students for embedded programming regarding the on-board computer. Control systems students to do ADCS design. From physics, students for orbital mechanics and defining the satellite trajectory and the radiation environment. Students from material science (physics and/or chemistry and/or chemical engineering) to design materials for passive radiation and thermal shielding among other innovative material research to increase functionality per unit mass.
This approach has the potential to simultaneously produce immediately practical and useful (perhaps marketable) research outputs across all involved disciplines in record time. It also creates an environment where even the most fundamental research can find immediate practical usefulness in addressing real-world problems.

Keywords: Education, Space applications, Concurrent research design, Concurrent engineering

Fostering Renewable Energy Research Collaborations Between U.S. and African Universities

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Renewable energy is the future of inclusive electricity access in Africa; thus, it is crucial to develop the education that fosters young engineers and scientists to advance the technology. The SciBridge project aims to promote research collaborations on emerging materials for sustainable energy between U.S. and African university students. The organization is based at North Carolina State University in Raleigh, North Carolina, U.S. and Makerere University in Kampala, Uganda and involves collaborations with multiple universities in both the U.S. and Africa. SciBridge provides participating students with kits that contain the lesson plan and equipment needed to perform novel experiments about materials for sustainable energy. Each kit contains enough supplies for 40 students and is sent to ten partner universities in four different African countries – Uganda, Ethiopia, Tanzania, and Rwanda. Since 2014, SciBridge has sent a total of 35 experiment kits on dye-sensitized solar cells, Al-air batteries, and thermoelectric generators. Examples of how these kits are used by our partners include classroom and workshop lessons, outreach programs with global businesses, senior design projects on solar cell efficiency simulations, and master's thesis research on dye-sensitized solar cells. Currently, SciBridge is developing new experiment kits, lesson plans, and tutorial videos based on topics that include a microbial fuel cell, a technology that harnesses electricity from bacteria, and a low-cost potentiostat, a device used to characterize electrochemical systems. Through our pen-pal program, undergraduate students in Africa and the U.S. collaborate by designing future experiment kits, networking, and sharing experiences. SciBridge believes conducting hands-on experiments will encourage students to pursue further studies in materials for renewable energy technologies and engage in Africa-U.S. research collaborations.

Keywords: Sustainability, Education, Renewable energy, Hands-on learning, Collaboration

Analysis of the Barriers That Limit the Development of Biogas in West Africa: Cross-Analysis in Senegal and Benin.

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The issue of supplying rural households with sufficient quality and quantity of domestic fuels is a major challenge in West Africa, particularly in Senegal and Benin.
This article deals with the reasons that explain the constraints that hinder, in Senegal and Benin, the development of the market for domestic biodigesters.
It first presents the energy and socio-economic profiles of the two countries by presenting the secondary data collected in the reports of the energy information systems as well as the national statistical data. By keeping this same approach, it shows the environmental consequences induced by the predominance of biomass as a source of cooking energy supply by referring to national communications on climate change.
Then, it includes a bibliographical review giving the state of the art in West Africa, particularly in Senegal and Benin. Indeed, the results of the work of scientific articles and doctoral theses, in particular the work of (CSE, 2019), (Cesaro et Al, 2021), (Cissokho et Al, 2019), (Gloria, 2018), (Kindomihou et Al, 2007), (Klein et Al, 2014), (Litzow et all, 2020), among others are visited. Results of field surveys carried out during the evaluation of Senegal's national domestic biogas program in 2014 and 2020 will also be called upon. Recent surveys carried out in July 2022 in Benin by the non-governmental organization Energy4Impact also show similarities in the trends related to the problem.
The singularity of this study lies in the cross-referencing of secondary data and data from diachronic field surveys revealing imbalances between the factors linked to livestock management, agriculture, pastoralism, sociology, economy and sustainable management of a domestic biodigester. Finally, sketches of solutions are presented.

Keywords: Anaerobic digestion, biodigesters, livestock, agriculture, pastoralism, organic matter, water, income, greenhouse gases

Active Learning Deconstructed – Bridging the Gap Between Engineering Professionals & Rural and Underrepresented Young Minds

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Engineering education and youth outreach has become a vital aspect of diversifying and developing STEM (science, technology, engineering, and math) fields especially following the effects of the pandemic. Even prior to the pandemic throughout the world, the widening gap between engineering professionals, collegiate level engineering students, science-oriented youth in wealthier areas/countries and youth lacking STEM exposure due to impoverished/ underrepresented backgrounds has been alarming. Active learning methods can connect and bridge the gap between each of these cohorts. Herein, we will discuss different techniques and practices for developing active learning activities with the incorporation of peer and professional mentoring for a variety of topics in materials science engineering. This integration will be further detailed in the Kenya Girls in STEM Program currently in development with Rutgers University and Hitaji Development Initiative. We will examine some of the takeaways from our initial workshop and areas of focus moving forward for future success. The provisional stages of a summer camp STEM program in conjunction with Colorado School of Mines and Tunza Sports Academy in Kenya will also be described.

Keywords: Youth Outreach, STEM Education, Mentoring



ORAL
PRESENTATERS

Research and Teaching Approaches in Material Science and Engineering in a Developing Country – Reflections of Early Career Researchers

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Material Science and Engineering is an enabler and driver of the technologies of the future. It is also critical to the important fields of Biotechnology and Information Technology, which underpins the Fourth Industrial era. As an early career researcher, my research interests are driven by current hotspots at the intersection of physical metallurgy, materials science, artificial intelligence and manufacturing. Thematic areas are rational alloy design (complimentary applications of computational and Edisonian approaches) of complex concentrated alloys for structural and functional applications, additive manufacturing and material repair using cold spray technologies. The concept of "dirty alloys", using scraps for next generation structural and functional alloys to fulfil the circular economic model is also being explored in a more sustainable way and at low-cost. Emphasis is on understanding mechanical, physical and chemical behaviour of these bulk materials and coatings. In terms of teaching and advising students at the undergraduate level, emphasis is on understanding fundamental concepts deeply, problem identification and problem-solving through rigorous idea generation sessions. For the Masters degree, where emphasis is on "mastery", our students are trained to understand the nature and purpose of the research, critiquing relevant literature while applying the right methodologies and techniques, and then ensuring a deeper appreciation of the consequence of the research findings. At the PhD level, finding a niche area, closing a gap in knowledge, helping students develop an independent critical judgment to generate novel or original ideas are necessary. This is done in collaboration with seasoned academics and industry experts in developed and developing countries leveraging the strength.

Understanding Students Learning Experience in Materials Science and Engineering by Using a Simple Conceptual Model to Analyse Critical Incidents

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To develop core pedagogical competence, teachers in higher education must be able to identify the core elements that influence students learning. Additionally, understanding the interactions between these critical elements would make teaching approaches to be centred on students learning. In this study, a simple conceptual model was developed by identifying the critical elements that influence students learning. The conceptual model comprises of elements that can either enhance or hamper learning. Learning theories were considered as elements that enhance learning, while learning barriers, cognitive overload, and alienation were taken as elements that negatively affect learning. The model was then based on the assumption that the core elements are a function of time, and their interactions are summative. This model was then used to analyse two critical incidents involving undergraduate students of metallurgical engineering. From this analysis, it was established that using a combination of learning theories while preventing learning barriers, alienation and cognitive overload could enhance the learning experience of students. Further work is considering the incorporation of assessments into the conceptual model.

Keywords: Learning theories; Learning barriers; Cognitive Overload; Higher Education.

Education as the Nexus for Technical and Societal Change: Innovative Data Informed Curriculum Design for 21st Century Materials Science and Engineering Teaching

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Africa is wealthy in natural resources, with approximately one third of the world's mineral reserves and is amongst the global leaders in minerals contributing to global innovation and technical change in fast-growing industries such as communication (cellular phones), transport (electric vehicles), and renewable energy. Africa is a youthful continent, with ~70% of the population of sub-Saharan Africa under the age of 30. Thus, education via metallurgy, mining, material science engineering, manufacturing, innovation and entrepreneurship, seats at the nexus between the young population and the natural wealth. This offers a catalyst for greater capitalisation of the youthful population in this 21st century. Education as the nexus for technical and societal change has shaped my career as a researcher in materials engineering and manufacturing, lecturer in teaching of Material science courses, and the director of academic development focusing on curriculum design. My research is the fields of advanced cermets and ceramics, surface engineering using laser technology (nano – femto), and additive manufacturing for functional and structural applications in automotive and aerospace industries. My teaching philosophy is, "taught content should apply to student's context and reality" (context-centred learning). To teach this effectively, one should apply a combination of consistently evolving educational and data-informed practices to facilitate learning and alleviate barriers (academic, eco-social and psycho-social) to student academic success. This philosophy was adopted in the curriculum design for the engineering common first year program, catering for ~1000 students from nine engineering disciplines, engineering course interventions as well as undergraduate and postgraduate student support. Lastly, innovative teaching technology (leveraging lessons learned during the COVID-19 pandemic) can significantly and cost-effectively improve access to education and training. This has been evident in the material and life science microscopy training of over 2000 postgraduate students, researchers, applied scientist and microscopists from over 200 institutions from 26 African countries.

Keywords: Nexus, Materials Engineering and Manufacturing, Societal good, Education, Learning technology

The Joint Undertaking for an African Materials Institute (Juami) Life Cycle Assessment Project

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Social, environmental, and economic life cycle assessments (LCA) have become critical decision-making tools in academia, industry, and government the world over. Materials LCA education has similarly become more common and best practices for teaching methodologies are in continuous development. This project is focused on a peer-to-peer mentorship model for LCA education in which PhD students in East Africa and the United States work together to develop and execute a comprehensive LCA to assess the sustainability of a local product or system. Specifically, the three pilot projects thus far have focused on biodiesel production in Uganda, the dairy industry in Tanzania, and the municipal solid waste system of Arusha, Tanzania. The model relies on vetted learning modules, developed at the Center for Socially Engaged Design (CSED) at the University of Michigan, that step the students through the process of goal and scope identification, inventory creation, and impact assessment. This is coupled with close mentorship and support from students who have previously conducted LCAs, live and virtual day-long LCA workshops, and access to an open, high computing power server with best-in-class LCA software as well as critical databases such as EcoInvent and the Social Hotspot Database. This combined approach of peer-to-peer mentorship curated educational materials and support, and access to critical computational infrastructure has proven to be successful in the implementation of the above-mentioned projects, with several currently under review for publication. We believe this model of a community-learning based approach to LCA education can be applied in other areas of the world to help train the next generation of global sustainability practitioners and educators. This project is supported by the National Science Foundation Joint Undertaking for an African Materials Institute (JUAMI) as well as the United Nations Environment Program (UNEP).

Keywords: life cycle assessment, education, virtual, material sustainability



POSTER
PRESENTERS

Collaborative Networking as a Bridge Between Innovation and Entrepreneurship

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The continuous discovery of new knowledge facilitated by science research breeds new innovations and one gateway for these innovations to be employed in society is through entrepreneurship. While the relationship between innovation and entrepreneurship has been proven Africa is yet to define its own parameters on how best this relationship can be salvaged to catalyze economic growth while ensuring that the integrity of research is not lost to commercialization. This work proposes the exploration of collaborative networking as a model that can be used to build a framework that efficiently facilitates the relationship within the African R&D eco system. The research will be carried out using an investigative methodology where case studies of both developing and developed countries will be analyzed. Important factors including, population size, availability of research facilities, access to funding and education systems will be considered.


Thank you!