NITheCS
National Institute for
Theoretical and Computational Sciences

NITheCS MINI-SCHOOL:

Energy Materials

Attend online: Wednesday 8, 15, 22 & 29 November 2023 | 14h00–15h00 SAST

ABSTRACT:

This mini-school discusses selected topics related to materials science and their applications in energy conversion. The first lecture will discuss the significance and unique properties of 2D materials for photocatalysis and photovoltaics along with the importance of 2D heterostructures for enhancing these applications. In the second lecture, current challenges in rechargeable batteries and fuel cells will be discussed and how computational tools can be used to improve conductivity and efficiency. The third lecture will focus on graphene-based catalysts for fuel cells and how computational tools can be employed to discover novel materials for high-capacity energy conversion. The school will conclude with a lecture that introduces the application of photosynthetic principles for designing efficient solar energy systems, with a focus on organic polymer solar cells and dye-sensitised solar cells.

LECTURE 1 (8 Nov)

'2D materials and their heterostructures for photocatalytic water splitting and Photovoltaics' – Prof Georgies Alene (Addis Ababa University, Ethiopia)

2D materials are atomically thin layers of materials that exhibit unique physical and chemical properties. They have attracted great attention for various applications, especially in the fields of photocatalysis and photovoltaics. Photocatalysis is the process of using light to drive chemical reactions, such as water splitting to produce hydrogen and oxygen. Photovoltaics is the conversion of light into electricity using semiconducting materials. In this lecture, I will introduce some of the 2D materials that have been used as photocatalysts and photovoltaics. I will also discuss how 2D heterostructures, which are combinations of different 2D materials, can enhance the performance of photocatalysis and photovoltaics. I will present some examples from my research work on computational study 2D heterostructures for photocatalytic water splitting and photovoltaics and highlight the challenges and opportunities in this emerging field.

LECTURE 2 (15 Nov)

'Overcoming Conductivity and Overvoltage Challenges in Rechargeable Metal-Ion and Metal-Air Batteries: Insights from DFT+U Studies' – Prof Yedilfana Setarge Mekonnen (Addis Ababa University, Ethiopia)

Rechargeable batteries have gained enormous attention for their versatile applications across various scales. However, challenges related to cost, recyclability, conductivity, and efficiency persist. To address some of the scientific challenges, we employed state-of-the-art density functional theory with the Hubbard U correction (DFT+U) tool. Unlike the pristine bulk phase, lattice-strained phases and surfaces of M2MnSiO4 (M=Li and Na) revealed good stability and fast ion transport, leading to enhanced conductivity and overall battery performance. Moreover, we examine the role of cathode-electrolyte interfaces on the ionic and electronic transport properties at the oxygen electrode in nonaqueous Li- and Na-air batteries. Furthermore, our research highlighted the effect of CO2 contamination on Li2O2, NaO2, and Na2O2 growth/depletion reaction pathways and overpotentials. Addressing the conductivity of electrodes and cathode-electrolyte interfaces is thus critical in the development of rechargeable batteries.

LECTURE 3 (22 Nov)

'Computational Modelling using high performance computing for materials prediction and design' – Dr Kingsley Obodo (North-West University)

The broad overarching aim of this presentation is to discover novel materials suitable for high-capacity energy conversion using density functional theory (DFT) calculations and advanced computational screening techniques. This discourse delves into the application of high-performance computing across various materials-centric projects, highlighting its pivotal role in facilitating materials prediction and design to promote sustainable advancement. The presentation will consider 2D materials, heterostructures as well different surface modelling based on Pt catalyst. 2D materials and heterostructures as possible photocatalytic materials as well as photovoltaic materials are discussed. We found that certain materials resulted in improved photocatalytic and photovoltaic properties. The reduction of platinum group metal towards the catalytic dehydrogenation of liquid organic hydrogen carriers (LOHC) is important due to the following consideration: materials perspective, commercialization, and cost implication. Thus, Pt based Sn alloys as well as Pt modified surfaces were explored and found to have better dehydrogenation catalytic properties compared with pristine Pt metals resulting in cost reduction attributed with reduced Pt loading. Also, the evaluation of doped IrO2 surface for oxygen evolution reaction (OER) underscores the potential to achieve elevated catalytic proficiency.

LECTURE 4 (29 Nov)

'Biological, biomimetic, and organic renewable solar energy materials' – Prof Tjaart Krüger (University of Pretoria)

The idea of using the principles underlying photosynthesis to design systems for making solar fuels has been around for over a century. The molecular machinery used by photosynthetic organisms demonstrates remarkably efficient and economical use of abundant natural elements for diverse applications in an extraordinarily fine-tuned and regulated fashion. The complex details of the photosynthetic processes are now known at a sufficient level that we can draw inspiration from them to improve the design of solar energy systems. In this lecture, I will discuss a few formidable design principles of photosynthetic light-harvesting complexes that may be used to improve the stability and performance of photovoltaic materials, focusing in particular on organic polymer solar cells and dye-sensitised solar cells.

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BIOGRAPHIES

Georgies Alene

Dr Georgies Alene is an associate professor at the Center for Materials Engineering in Addis Ababa Institute of Technology, Addis Ababa University, Ethiopia. He is currently the head of Center for Materials Engineering. He has a BSc in Applied Physics from Arba Minch University, Ethiopia (2003-2006), an MSc in Materials Science and Engineering from Augsburg University, Germany, and Grenoble Institute of Technology, France (2008-2010), and a PhD in Electrical Engineering (Electronics Materials and Devices) from Oulu University, Finland (2014-2018).
He has also worked as a graduate assistant (2006-2008) and a lecturer (2010-2014) in the Department of Physics at Arba Minch University, Ethiopia. His research interests include 2D materials and their heterostructures for photocatalytic water splitting and photovoltaics, synthesis and characterization of nanomaterials, nanodevices, DFT study of 2D materials, and energy efficiency for facilities.
He has published several papers in international journals and conferences and received grants for his research excellence. He is also actively involved in teaching, mentoring and supervising graduate students at Addis Ababa University.

Yedilfana Setarge Mekonnen

Dr Yedilfana Setarge Mekonnen is an Associate Professor in Energy Storage and Conversion Technologies at the Center for Environmental Science and Associate Dean for Graduate Programs at the College of Natural and Computational Sciences, Addis Ababa University (AAU), Ethiopia. He obtained his PhD degree in 2015 from the Technical University of Denmark. He holds an MSc degree in Physical Chemistry from AAU. Dr Mekonnen has also conducted postdoctoral research in the USA, China, and Italy, and has been an associate member of the Abdu Salam International Center for Theoretical Physics (ICTP) since 2020. He has led numerous research projects focusing on rechargeable batteries, fuel cells, solar cells, and bioenergy. He has received multiple research grants and awards. He has supervised over 25 graduate students at AAU and published over 36 papers in esteemed international journals. Additionally, he is the president of the Computational Science and Engineering Society of Ethiopia (CSESE) and holds the position of Vice President of the Chemical Society of Ethiopia (CSE).

The primary focus of his research is in the field of computational materials science, particularly utilizing tools such as density functional theory, molecular dynamics simulation, and machine learning. His studies mainly emphasize structural and electronic properties, reaction mechanisms, charge transport phenomena in various electrode materials used in rechargeable metal-ion batteries, metal-air batteries, proton exchange membrane fuel cells, and dye-sensitized solar cells, as well as catalysts for biodiesel production.

Kingsley Obodo

Dr Obodo is a Computational Scientist in HySA centre of competence at North-West University. His background is in ab initio (computational) modelling of various materials, with key interests in the application of physics, materials science, philosophical thinking towards innovations in energy and materials solutions, as well as research, design and development towards sustainability.

Dr Obodo has authored and drafted several technical reports for different projects in addition to numerous publications in peer-review journals. He has over 10 years of experience in research and development, with expertise in scientific programming languages. He plays roles in various projects that have deployed quantitative and qualitative research output, as well as applied these to problems in education, ICT, business and social science among others. He also has several local and international collaborations and is actively engaged in student supervision and mentoring.

Tjaart Krüger

Prof Tjaart Krüger is an Associate Professor in Physics at the University of Pretoria. He completed his PhD and a postdoctoral fellowship at the Vrije Universiteit in Amsterdam. He is passionate about multidisciplinary research and interested in the molecular details of energy transfer and regulation in various photosynthetic organisms' light-harvesting complexes and how the underlying principles may be applied to improve the design and performance of solar cells. His research involves various laser spectroscopy techniques and theoretical and computational approaches and has been published in nearly 60 journal articles and acknowledged through several awards.

He has a broad international collaborative network and has supervised over 15 postgraduate students to completion. He is a former executive committee member of the South African Young Academy of Science (SAYAS), chair of the South African Biophysics Initiative, and a senior editor of the prestigious *Journal of Physical Chemistry Letters*.