A*STAR – NUS MSE JOINT WORKSHOP

ON EMERGING TECHNOLOGIES FOR ENVIRONMENTAL SUSTAINABILITY

15 Dec 2020, Tuesday, 0900 – 1230

*Jointly brought to you by NUS MSE, A*STAR IMRE, IHPC and SIMTech*

Programme:

Time	Content
0905 – 0925	**Welcome Address** (Moderator: Dr LI Zibiao, IMRE) • Prof Barbaros OEZYILMAZ, Head, NUS MSE • Prof LOH Xian Jun, Executive Director, A*STAR IMRE
0930 – 1050	**Part 1: CO_2 Capture and Conversion** (Moderator: Dr LEONG Zhidong, IHPC) • *New opportunities in CO_2 capture and conversion using electrochemistry* by Asst. Prof Andrew Barnabas WONG (NUS MSE) • *Transforming waste CO_2 into renewable chemicals and fuels* by Dr LUM Yanwei (A*STAR IMRE) • *First-principles-based catalytic modelling in CO_2 conversion and H_2 production* by Dr ZHANG Jia (A*STAR IHPC) • *New Membrane for Non-aqueous and Gaseous Molecular Filtration for Sustainability* by Dr DONG Xuecheng (A*STAR SIMTech)
1055 - 1215	**Part 2: Materials for Batteries and Electrocatalysis** (Moderator: A/Prof ADAM Shaffique, NUS) • *Redox-mediated Electrochemical Energy Conversion and Storage* by A/Prof WANG Qing (NUS MSE) • *Nanostructured Materials for Batteries and Fuel Cells* by Dr LIU Zhaolin (A*STAR IMRE) • *Alloy Design for Energy Applications via High-Throughput DFT and Machine-Learned Surrogate Models* by Dr TAN Teck Leong (A*STAR IHPC) • *Life Cycle Assessment (LCA): A tool for understanding sustainability attributes of products & systems* by Dr YEO Zhiquan (A*STAR, SIMTech)
1220 – 1230	**Closing Remarks**

The online workshop may be accessed via Zoom:

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Abstracts and Biographies of Presenting Speakers

Asst. Prof Andrew Barnabas WONG (NUS MSE)

New opportunities in CO_2 capture and conversion using electrochemistry

Biography:

Andrew B. Wong is an assistant professor at the National University of Singapore in the Material Science and Engineering Department with a joint appointment in the Chemical and Biomolecular Engineering Department. He received a joint B.S.-M.S. in Chemistry at the University of Chicago in 2011, and he received his Ph.D. in Chemistry at the University of California Berkeley under the mentorship of Prof. Peidong Yang. His Ph.D. research focused on the synthesis and characterization of nanostructured solution-processed semiconductors. After working with Prof. Thomas Jaramillo at Stanford University in electrocatalytic CO_2 conversion, he began his independent career at NUS in 2020. His current research interests include electrocatalysis, electrosynthesis, and developing new materials and processes for sustainable energy technologies.

Abstract:

With the urgent need to develop new technologies to capture, store, and utilize CO_2, electrocatalysis has been vigorously investigated as a potential approach for CO_2 conversion to fuels, chemical feedstocks, and structural materials. While significant progress has been made in the last decade, new approaches are still urgently needed to develop the enabling technologies that will lead to economically feasible CO_2 capture and conversion. To develop these enabling technologies, this talk will discuss the basis for exploring the electroreduction of CO_2 to C in molten salt electrolytes to form value-added products such as carbon nanotubes. In addition, this talk will discuss the potential of this molten salt approach to address many of the key challenges that are currently faced by lab-scale GDE-based and MEA-based approaches to CO_2 electroreduction. These challenges include long-term stability, impurity tolerance, faradaic efficiency, conversion efficiency, and product value. Furthermore, this talk will also survey the potential for new processes for CO_2 capture based on electrochemical steps focused on electrochemical regeneration of capture media or by performing electrocatalysis on captured and bound CO_2 equivalents. Overall, the development and implementation of new, enabling CO_2 capture and conversion technologies will require highly collaborative and interdisciplinary efforts, and the development of these technologies will be transformative on a global scale at scientific, environmental, and economic levels. In the long-term, the collaborative development of these new technologies will enable global society to be more carbon neutral and sustainable.

Assoc Prof WANG Qing (NUS MSE)

Redox-mediated Electrochemical Energy Conversion and Storage

Biography:

Dr. Qing Wang is an Associate Professor at the Department of Materials Science & Engineering, National University of Singapore. His research interest is “Charge Transport in Mesoscopic Energy Conversion and Storage Systems”. Based on the redox targeting concept, his group is extensively working on a new battery technology — redox targeting-based flow batteries and beyond, with the implementations to a wide variety of battery chemistries for advanced large-scale energy storage.

Abstract:

Redox reaction involving charge transfer at the electrode-electrolyte interface represents an essential process for various electrochemical energy conversion and storage applications, such as fuel cell, electrolyzer and battery, etc. As a result, the operation (i.e. cell voltage, current density, turnover number, etc.) of the above devices is inherently dictated and constrained by the redox reactions. The redox-mediated process, a chemical reaction between an electrolyte-borne redox species electrochemically generated on electrode and a material (generally insoluble in electrolyte) off the electrode, provides additional flexibility in circumventing the constraints intrinsically confronted by the conventional electrochemical devices. One example is the redox targeting of energy storage materials for flow

batteries. The redox-mediated reactions of high capacity solid material stored in the tank with redox electrolyte flowing through it considerably boost the energy density of redox flow battery without compromising its operation flexibility. Another example is redox-mediated oxygen evolution reaction (OER) for water electrolysis. The concurrent electrochemical-chemical cycle enables continuous reaction between an electrolyte-borne redox mediator and an OER catalyst loaded in a fixed-bed reactor spatially separated from the cell, which is believed to be advantageous to enhanced gas purity and safety. In this talk, I will report our latest advancement in the above area. In addition, I will briefly introduce some other studies on redox-mediated reactions, such as low-grade waste heat harnessing based on a thermal-electrochemical cycle and battery material recycling based on a one-way redox targeting reaction.

Dr LUM Yanwei (A*STAR IMRE)

Transforming waste CO_2 into renewable chemicals and fuels

Biography:
Dr. Lum Yanwei received his PhD in Materials Science & Engineering at the University of California, Berkeley in 2018. His studies were funded by an A*STAR National Science Scholarship and focused on electrocatalytic CO_2 conversion. Following this, he performed postdoctoral work at the University of Toronto, engaged in electrochemical hydrocarbon valorization using an integrated theoretical and experimental approach. Presently, he is a Group Leader at the Institute of Materials Research & Engineering (IMRE). His awards include a KAUST Industry Collaboration Program's Young Speaker Award (2018), an A*STAR Career Development Award (2020) and an NTU-SNIC Oral Presentation Award (2020).

Abstract:
Efficiently recycling CO_2 waste into value-added products presents a significant challenge towards realizing a sustainable energy future. An attractive strategy uses renewable electricity to electrochemically convert CO_2 into chemicals and fuels - just like photosynthesis, except at a much-accelerated pace. At the heart of this process are electrocatalysts, which mediate electron transfer and facilitate these conversion reactions. In this talk, I will first provide an introduction to electrochemical CO_2 conversion and motivate this as a promising pathway for decarbonization of chemical production.
Next, I will give a short overview of my research in this burgeoning area, including novel isotopic approaches for uncovering mechanistic insights[1,2], designing model electrocatalytic systems[3] and the effect of metallic oxide-based reaction modulators[4]. In addition, I will briefly describe how renewable ethylene generated by such a process can be further electrochemically upgraded into valuable plastic precursors[5,6]. Finally, I highlight my future work and plans in this exciting and important area of research.

[1] Y. Lum and J.W. Ager. *Angewandte Chemie* (2018) 57 (2), 551-554
[2] Y. Lum and J.W. Ager. *Nature Catalysis* (2019) 2 (1), 86-93
[3] Y. Lum and J.W. Ager. *Energy & Environmental Science* (2018), 11 (10), 2935-2944
[4] Y. Li#, A. Xu#, Y. Lum# and E. H. Sargent et. al. *Nature Communications* (2020), Accepted.
[5] Y. Lum#, J.E. Huang#, Z. Wang and E. H. Sargent et al. *Nature Catalysis* (2020) 3 (1), 14–22
[6] W.R. Leow#, Y. Lum#, A. Ozden and E. H. Sargent et al. *Science* (2020), 368 (6496), 1228-1233

Dr LIU Zhaolin (A*STAR IMRE)

Nanostructured Materials for Batteries and Fuel Cells

Biography:
Dr Liu Zhaolin is a Senior Scientist III at IMRE, A*STAR. His current research interest includes design, synthesis, and structural studies of energy storage materials and development of novel nanostructured materials which are suitable to be applied in Li-ion and metal-air batteries, and their prototyping. His research interest also includes fuel cell catalyst and membrane. He has published more than 204 research papers in refereed scientific journals and received a total citation of more than 14,000 with h-index of 66 (Web of Science). He has secured and completed 16 industry projects with RCA as project leader, total project cost is more than $5.6 million.

Abstract:
Nanostructured materials are currently of interest for batteries and fuel cells because of their high surface area, novel size effects, significantly enhanced kinetics, and so on. The presentation will describe some our works in nanostructured anode and cathode materials for lithium-ion batteries, I will discuss how to further develop electrode materials, electrolyte, electrode formulation, battery design engineering in Li-ion batteries. I will also give a brief introduction for our research works on nanostructured electrocatalysts as air electrode for metal-air batteries, as well as nanostructured Pt-based electrocatalysts for proton exchange fuel cell (PEMFC) and direct methanol fuel cell (DMFC).

Dr ZHANG Jia (A*STAR IHPC)
First-principles-based Catalytic Modelling in CO_2 Conversion and H_2 Production

Biography:
Dr Zhang Jia is currently a Senior Scientist as well as Group Manager of Chemistry & Catalysts Group, in the Department of Material Science and Chemistry, Institute of High Performance Computing (IHPC), A*STAR, Singapore. Her current research interests are computational heterogeneous catalysis and material chemistry of solid catalysts. She is a Co-I for the Accelerated Catalyst Development Platform and PIPS projects on catalysis in addition to leading industry projects with international catalyst and chemical companies. Her research work has been published in top journals including ACS Catal., Angew. Chem. Int. Ed., J. Am. Chem. Soc., and Nano Lett.

Abstract:
Computational modelling is a powerful tool to understand reaction mechanism and provide insights in rational catalyst design. The Chemistry & Catalysts Group in IHPC has strong expertise in both computational heterogeneous catalysis and homogeneous catalysis. We have worked in a variety of areas from thermal catalysis to electrocatalysis; from transitional metal surface to multi-metal oxide; from nanoparticles to single-atom catalyst. Currently, our catalysis research focuses on topics associated with environmental sustainability, and important reactions in chemical and pharmaceutical industries. In this talk, we will give an overview of the Chemistry & Catalysts Group and share a couple of examples on our recent research, e.g. CO_2 conversion to syngas and selective dehydrogenation of formic acid to generate H_2.

Dr TAN Teck Leong (A*STAR IHPC)
Alloy Design for Energy Applications via High-Throughput DFT and Machine-Learned Surrogate Models

Biography:
Dr. Tan Teck Leong obtained his PhD from the University of Illinois Urbana-Champaign in the area of computational materials science. Currently, as a senior scientist and deputy department director in the Materials Science & Chemistry Department in IHPC, he is leading multi-disciplinary use-inspired research in the area of alloy materials design with the aim of accelerating materials development in the areas of aerospace, nanoscale technology, catalysis and electronics. He enjoys algorithm development and is building platforms to help bridge physics-based simulations with machine-learned models to increase the throughput of material property predictions.

Abstract:
Nanoscale alloys are actively explored in clean-energy research as electrocatalysts, photocatalysts and batteries. By mixing of two or more elements, alloying, offers an avenue to tune functional properties of materials. First-principles density functional theory (DFT) calculations has proven to be a reliable tool for electrocatalysts and battery materials design, by providing fundamental chemistry insights into the reaction and intercalation mechanisms. However, for alloy design, the prediction will only be accurate provided the correct material structure is given as the input for the first-principles calculations. To this end, we couple first-principles calculations with machine-learned physics-based surrogate models, such as the cluster expansion method, to realize a cost-effective avenue to identify stable nanoscale structures. Using the effective atomistic interactions created from first-principles, one could perform an

efficient sweep over millions of possible alloy configurations/structures and via Monte Carlo simulations to design stable alloy structures with the desired (electro)catalytic properties. After a brief introduction to the alloy design methodologies, I will showcase some of our recent applications to the electrochemistry modelling of alloy nanoparticles and surfaces as well as the characterization and prediction of the properties of battery electrode materials.

Dr DONG Xuecheng (A*STAR SIMTech)

New Membrane for Non-aqueous and Gaseous Molecular Filtration for Sustainability

Biography:

Dr Dong Xuecheng is a Scientist and Section Manager of the Sustainable & Symbiotic Production Technology (S^2PT), under Sustainability and Life Cycle Engineering (SLE) Group. Over 8+ years in A*STAR SIMTech, he initiates and manages academic and industrial research projects, e.g. projects under Pharma Innovation Programme Singapore (A*STAR PIPS) and projects under Singapore Aerospace Programme Consortium (A*STAR SAP) with focus on sustainability, close-loop continuous manufacturing, lightweight and corrosion protection, as well as projects sponsored by public trust fund, local and overseas universities with total research fund more than SGD 2 mil.

As a Research Scientist in material science, thin film, interface, and membrane, Xuecheng has developed technology portfolio for waste valorization and material sustainability, e.g. recovering and regenerating aqueous and non-aqueous waste stream, surface treatment processes for metal and light weight alloy corrosion protection, and aerospace MRO. Xuecheng is a certified trainer and conducts SSG's Workforce Skills Qualification (WSQ) module over the past 8 years.

As a Section manager of S^2PT, Xuecheng coordinates the team research effort to provide solutions to companies, which express short term urgent needs in material and waste issues; meanwhile he strategises the team research roadmap to develop new sustainable technologies and symbiotic supply chains with collaborators for Singapore industry to achieve close-loop manufacturing and circular production in long term.

Abstract:

The reduction of waste from chemical processes is becoming a strong focus in many industries towards a green and sustainable circular economy. Many researches are addressing the end-of-pipe treatment to the elimination of wastes at the source at the same time a sound internal recycling. New strategies based on the hierarchical process design have been developed and used in the practice. In the case of a chemical company that consists of several processes or plants it is necessary to co-ordinate the waste minimisation incentives on the company level. The main aim is to evaluate the waste between processes to design close-loop processing. New methods of micro-, nano-level separation are those emmerging key pillars to contribute towards an effective waste treatment. Membrane technology has enabled cost-effective process separations of mixtures, applied to aqueous, solvents and gaseous streams, both in terms of purification, separation and fractionation of, valuable materials/product reuse, recovery, and recycle.

To date, polymeric membranes in hollow-fiber and spiral wound (flat-sheet) configurations have dominated the membrane market with 90% or more of the installed industrial capacity. While polymeric membranes have functioned well in water applications, they are very limited in achieving more difficult separations involving complex mixtures, performed under more extreme conditions that may pose a risk to the polymeric material nature (e.g., high temperature- or solvent-induced failure).

SIMTech's novel membranes can provide a number of significant advantages over polymeric membranes in terms of process and material robustness, reliability. Together our process technology, SIMTech's membrane for non-aqueous and gaseous molecular filtration can support many industry sectors, such as pharma, biomedical, food & beverage, petrochemical/hydrogen, etc. to improve resource circularity and manufacturing sustainability, while reduce carbon foot print and waste.

Dr YEO Zhiquan (A*STAR SIMTech)

Life Cycle Assessment (LCA): A tool for understanding sustainability attributes of products & systems

Biography:

Dr. Yeo Zhiquan is the Deputy Group Manager of the Sustainability and Life Cycle Management Group at A*STAR SIMTech and concurrently oversees a research section in the academic discipline of Industrial Ecology. Over the past ten years, he has been actively involved in industry and research projects that promotes industrial sustainability, ranging from Life Cycle Assessment (LCA) studies to data science applications for enabling industrial symbiosis and circular economy activities. Zhiquan is also currently appointed as the Singapore representative for the Sustainability Certification Scheme Evaluation Group supporting the Committee on Aviation Environmental Protection (CAEP) of International Civil Aviation Organization (ICAO).

Abstract:

With growing attention placed on the topic of sustainability, technological solutions addressing sustainability challenges have also gained momentum. In applying technologies to address various environmental issues, a potential pitfall is the phenomenon of problem-shifting – whereby one environmental problem is solved while creating unintended consequences in other parts of the value chain or system. To minimise the occurrence of such problem-shifting, a holistic life cycle perspective needs to be adopted whilst developing or deploying sustainable technology solutions. Life Cycle Assessment (LCA) serves as a tool to help operationalise this life cycle perspective and thinking, wherein it provides quantitative measures and indicators to guide decisions in the context of developing and deploying sustainability oriented technologies. With LCA as the accompanying decision support tool alongside technology development, sound evidence-based decisions can be made to progress towards truly sustainable solutions.

This online workshop is open to all and is jointly brought to you by NUS Department of Material Science Engineering (NUS MSE), A*STAR Institute of Materials Research and Engineering (IMRE), A*STAR Institute of High Performance Computing (IHPC), and A*STAR Singapore Institute of Manufacturing Technology (SIMTech).

Organising committee:

- Dr LI Zibiao, IMRE, A*STAR (lizb@imre.a-star.edu.sg)
- A/Prof ADAM Shaffique, NUS (shaffique.adam@yale-nus.edu.sg)
- Dr TAN Teck Leong, IHPC, A*STAR (tantl@ihpc.a-star.edu.sg)
- Dr DONG Xuecheng, SIMTech, A*STAR (xcdong@simtech.a-star.edu.sg)

Kindly drop an e-mail to any of the above organising committee members if you have any queries regarding details of the workshop. We look forward to your keen participation.