CLEAN TECHNOLOGIES RESEARCH INSTITUTE

Student Symposium

Monday, August 23rd and Tuesday, August 24th, 2021

Teams Live Event

Organizing Committee

Ahmed Eldesoky, Department of Chemistry

Rania Elsebai, Department of Process Engineering and Applied Science

Reem Karaballi, Department of Chemistry

Roksana Saleh, Department of Plant, Food and Environmental Sciences

Preston Stronach, School of Architecture

Tina Taskovic, Department of Chemistry

CLEAN TECHNOLOGIES RESEARCH INSTITUTE

Student Symposium

Monday, August 23rd and Tuesday, August 24th

Teams Live Event

DAY 1, Monday, August 23rd

Chair: Tina Taskovic

12:30 – 12:40 pm **Welcome and Opening Remarks – Prof. Michael Freund**

12:40 – 1:30 pm **Dr. Elizabeth Mayo**
Vice President of Operations

Brookfield Renewable
From Grad Student to Vice President

1:30 - 1:50 pm **Patrick Giesbrecht**
Department of Chemistry
Improving the Analysis of Electrochemical Impedance Spectra of Vapor-fed Water Electrolysers using New Mathematical Transformations

1:50 - 2:10 pm **Conner Spence**
Department of Mechanical Engineering
Development of a Powder Metallurgy Counterpart to Aluminum Alloy 6063 Dalhousie

2:10 - 2:30 pm **Sammy Hanuka**
Department of Chemistry
Developing an EEC Model for Faradaic Reactions in Porous Supercapacitor Electrodes

2:30 – 3:40 pm **Break**

2:40 - 3:00 pm	**Roksana Saleh** Department of Plant, Food & Environmental Sciences ***The Effects of Natural Media Amendments on Growth Factors of Microgreens Cultivated in Indoor Production System***
3:00 - 3:20 pm	**Nick Gosse** Department of Mechanical Engineering ***Inter-vendor Study of Directed Energy Deposition Build Quality Using a Commercial Ti-64 Powder***
3:20 - 3:40 pm	**Ziyi Chen** Department of Chemistry ***X-ray Spectroscopy of Thiolate-Protected Silver Nanoclusters***
3: 40 - 4:00 pm	**Piper Sawchyn** Department of Chemistry ***Porous Electrode Materials: How Pore Shape Affects Performance***
4:00 - 4:05 pm	**Daily Wrap Up**
4:05 - 4:15 pm	**Break**
4:15 - 5:00	**Teams Meeting - Discussion Group 1 Electrochemistry (Giesbrecht, Hanuka, Sawchyn, *Moderator: Reem Karaballi*)**
4:15 - 5:00	**Teams Meeting - Discussion Group 2 Materials (Spence, Saleh, Gosse, Chen, *Moderator: Rania Elsebai*)**

Keynote Address

From Grad Student to Vice President

Dr. Elizabeth Mayo
Vice President, Operations
Brookfield Renewable

As Vice President of Operations, Elizabeth Mayo oversees asset performance, customer care and health, safety, security and environmental matters. She is responsible for optimizing generation, identifying repowering opportunities and working with existing customers on new DER opportunities.

Before joining Brookfield in 2020, Dr. Mayo was the Global Director of Solar Services at Underwriter's Laboratory, managing the Solar Consulting Practice for due diligence, energy services and asset management. Prior to that, she was Head of Department at DNV GL, where she managed the technical engineering teams and ran the operation of the PV Evolution Testing labs for modules, inverters and batteries.

Dr. Mayo holds a Bachelor of Science degree and a Master of Science Education degree from Florida State University, as well as a Ph.D. in Chemistry from California Institute of Technology.

Improving the Analysis of Electrochemical Impedance Spectra of Vapor-fed Water Electrolysers using New Mathematical Transformations

Patrick Giesbrecht
Chemistry

Email: pgiesbrecht@dal.ca
Co Authors: Michael S. Freund
Research Supervisor: Prof. Michael Freund

Water electrolysers allow the coupling of electricity from renewable sources to the generation of 'green' hydrogen from water. One electrolyser format, polymer electrolyte membrane water electrolyser (PEMWE), has garnered interest due to its compact design, high hydrogen generation rates. However, widespread adoption of PEMWEs has been limited due to material scarcity and low power efficiencies, where an understanding of the underlying performance losses and degradation pathways is necessary for future design and implementation. Electrochemical impedance spectroscopy (EIS) can provide such insight in situ and has become a key method for monitoring performance losses in fuel cells. However, current understanding of the impedance response of PEMWEs is still preliminary given the complexity of the system. Interpretation of the EIS response can be improved by using a recently developed method, distribution of relaxation times (DRT). DRT converts EIS data from the frequency domain to the time domain, allowing different processes to be separated based on their time constants. Here, DRT is used to analyze the operation of a vapor-fed PEMWE and determine the different contributions that result in performance losses under various conditions. Vapor-fed operation of a PEMWE allows analysis of the impact of water transport, electrode kinetics, and ionic resistances in the cell without interference by liquid electrolyte or product bubbles. From these analyses, an equivalent circuit model for vapor-fed PEMWE operation is developed, with areas for improvements and limitations discussed.

Optimization of Process Parameters and Sintering Aids for Press and Sinter of 6063 Aluminum

Conner Spence
Materials Engingeering
Email: conner.spence@dal.ca

6063 Aluminum is the most widely used Al alloy for extrusion applications and offers exemplary surface finish and ability to form complex shapes, while maintaining appreciable strength. In powder metallurgy applications it has the potential to offer great functionality as well, with the net-shape nature of the process allowing for increased material and energy efficiency in manufacturing. The present work is directed towards the use of this technique in producing complex shapes with maximized thermal conductivity in the finished parts. The work focused first on overcoming the expected hurdles in the press and sinter of aluminum powders to achieve appreciable densification. Specifically, small additions of tin and variations in sintering temperature and sintering time. The identification of ideal parameters at this stage has facilitated more in depth optimization work in the areas of sizing response, artificial aging characteristics, and the impact of all varied parameters on the thermal properties of the finished parts.

Developing an EEC Model for Faradaic Reactions in Porous Supercapacitor Electrodes

Sammy Hanuka
Chemistry

Email: sammy.hanuka@dal.ca
Co Authors: Heather Andreas
Research Supervisor: Prof. Heather Andreas

Porous supercapacitors provide a unique balance of power and energy-density by coupling a high surface area with highly reversible (fast) charge storage mechanisms. Unfortunately, supercapacitors can also suffer from irreversible faradaic reactions that limit their efficiency and cause self-discharge. It is often difficult to isolate the relative contribution of these processes, especially in porous environments, because pores experience non-uniform charge storage and redistribution along their surface. Since pores are difficult to characterize using conventional electrochemical experiments, equivalent electrical circuit (EEC) models have been developed to help further our fundamental understanding of porous charge storage. These EEC are often modelled virtually using simulation programs with integrated circuit emphasis (SPICE). Currently, de Levie's transmission line circuit (TLC) is used to model capacitance and charge movement inside pores; however, faradaic reactions are ignored. To date, faradaic EEC have only been modelled for planar surfaces, limiting their applicability towards the behaviour of porous electrodes.

This work is the first to use a TLC in order to model both faradaic reactions and capacitive charge storage together within an electrochemical pore. The EEC for both activation-controlled and diffusion-controlled faradaic reactions are incorporated as branches into each TLC segment, taking advantage of the TLC's ability to model incremental resistance. Circuits are characterized in SPICE through simulated cyclic voltammetry (CV) and evaluated against manganese oxide electrodes. The unified pore EEC model can help increase our understanding of the competing effects of capacitive and faradaic processes on charge storage within pores.

Natural Growing Medium Amendment Effect on Growth of Microgreens

Roksana Saleh
Plant, Food, Environmental Sciences,
Faculty of Agriculture, Dalhousie University

Email: rk286030@dal.ca
Co Authors: Dr. Lord Abbey
Research Supervisor: Dr. Lord Abbey

Microgreens are immature tender young plants grown and eaten for their high health-promotion and functional biological properties. Microgreens' response to growth factors is understudied. A study was carried out to evaluate the effects of different mixed growing media on the growth response of different microgreens plant species; namely, kale (*Brassica oleracea* L. var. *acephala*), Swiss chard (*Beta vulgaris* var. *cicla*), Arugula (*Eruca vesicaria* ssp. *sativa*), and Amaranth (*Amaranthus tricolour* L.). The experimental treatments were T1: 30% vermicast + 40% sawdust + 30% perlite; T2: 30% vermicast + 50%s awdust + 20% perlite; T3: 50% vermicast + 30% sawdust + 20% perlite; T4: 30% vermicast + 40% sawdust + 30% mushroom compost; T5: 30% vermicast + 20% sawdust + 20% perlite + 30% mushroom compost; NC: 50% sawdust + 50% mushroom compost, and PC: Pro-mix BX™ potting medium alone. It was shown that physicochemical properties of the different growing media varied. Salinity, total dissolved solids, electrical conductivity, and pH in T4 and T5 were higher than all the other treatments. Similar observations were made on T4 porosity (45.4%) and water retention (431.5 m^3/m^3). Besides, higher plant height was observed in PC and T5 for all the plant species. Germination percentage was higher in PC for all plant species, except for kale that was higher in T5. Thus, the present study suggested that T4 and T5 ameliorated growing media chemical properties better than the other treatments, hence the improved plant growth indices in these media. Overall, T5 was the most effective media for microgreen production. Future studies should consider the effects of natural mixed growing media on microgreens phytonutrients.

Keywords:plant growth, microgreens, natural amendment, preharvest factors.

Inter-vendor Study of Directed Energy Deposition Build Quality Using a Commercial Ti-64 Powder

Nick Gosse
Mechanical Engineering

Email: nick.gosse@dal.ca
Co Authors: Matthew Harding, Paul D Bishop, Ian W Donaldson
Research Supervisor: Prof. Paul Bishop

This research sought to compare the manufacturing capabilities of several vendors of directed energy deposition (DED) equipment in the context of additive manufacturing. Gas atomized Ti-64 powder was utilized in all instances as it maintains a high relevance to industrial practice and is readily applicable in DED processing. A single commercial lot of Ancor Ti-64 powder was secured for this purpose, characterized, and then distributed amongst multiple OEMs of DED equipment. Vendors were also given a 3D model and dimensioned drawing of the desired test build geometry. Upon receipt of the completed builds, dimensions of interest were measured using a 3D coordinate measurement machine and compared to the provided model. Builds were also compared based on a range of metallurgical assessments. These included the acquisition of data on hardness, density (MPIF Standard 42), and tensile properties (ASTM E8M). In addition, optical micrography, scanning electron microscopy, differential scanning calorimetry and x-ray diffraction were utilized to characterize microstructural features of each build.

X-ray Spectroscopy of Thiolate-Protected Silver Nanoclusters

Ziyi Chen
Chemistry

Email: ziyi.chen@dal.ca
Co Authors: Peng Zhang, Manzhou Zhu
Research Supervisor: Prof. Peng Zhang

Atomically precise metal nanoclusters have attracted significant interest due to their molecular-like properties and they can be applied in many fields. $Ag_{25}(SR)_{18}$ are one of Ag nanoclusters with determined total structure, which also are the only match analogues with Au nanoclusters, $Au_{25}(SR_{)18}$. In this presentation, the X-ray spectroscopy study of $Ag_{25}(SR)_{18}$will be presented. It will be demonstrated that the X-ray absorption spectroscopy (XAS) as a main tool can probe both the electronic and bonding properties of $Ag_{25}(SR)_{18}$from site-specific perspective. The unique analysis methods developed for the X-ray spectroscopy of $Ag_{25}(SR)_{18}$ can be applied to other nanocluster system to investigate the structure-property relationship.

Porous Electrode Materials: How Pore Shape Affects Performance

Piper Sawchyn
Chemistry

Email: pp527749@dal.ca
Co Authors: Heather Andreas, Sammy Hanuka
Research Supervisor: Prof. Heather Andreas

This work explores the effect that the shape of pores within porous electrode materials may have on some figures of merit used to judge supercapacitor performance. Some examples include charge/discharge capacity, energy density, and power. Charge redistribution, a phenomenon that occurs spontaneously to equalize potential gradients, was successfully demonstrated to be dependent on pore shape using transmission line circuit (TLC) modeling. Now, virtual TLC modeling via LTSpice is used to explore how total resistance, pore length, pore mouth diameter, and other factors inherent to pore shape affect supercapacitor performance. This project explores if certain shapes perform better overall, and/or if some shapes stand out as being better regarding individual parameters.

CLEAN TECHNOLOGIES RESEARCH INSTITUTE

Student Symposium

Monday, August 23rd and Tuesday, August 24th

Teams Live Event

DAY 2, Tuesday, August 24th

Chair: Reem Karaballi

12:30 - 12:40 pm **Welcome and Opening Remarks**

12:40 - 1:10 pm **Various Presenters**
Introductions to Organizations

1:10 - 1:30 pm **Sarah Martell**
Department of Chemistry

The Influence of HF Etching Process on the Photocatalytic H2 Evolution Reaction Using Mesoporous Si Nanoparticles

1:30 - 1:50 pm **Dylan Hale**
Department of Chemistry
Bis(phosphino)silyl Ni Hydride Catalyzed Alkyne Hydrogenation

1:50 - 2:00 pm **Break**

2:00 - 2:20 pm **Kathleen Walker**
Department of Engineering

Evolution of Environmental Sustainable Wood Preservatives

2:20 - 2:40 pm **Andrew Walsh**
Department of Chemistry
The Electronic Properties of Silver Nanoclusters as Determined Through X-ray Absorption Spectroscopy and Density Functional Theory

2:40 - 3:00 pm **Ryan Ley**
Department of Mechanical Engineering
Binder Jet Printing of Low-Cost Tool Steel Powders

3:00 - 3:20 pm **Pardis Pourmohammadi**
Department of Industrial Engineering
A robust simulation-optimization approach for designing hybrid renewable energy systems

3:20 - 3:40 pm **Zachary Simunovic**
Department of Mechanical Engineering
Laser Scanner for Cell Thickness Mapping and Volume

3:40 - 3:45 pm **Wrap up**

3:45 - 4:00 pm **Break**

4:00 - 5:00 pm **Teams Meeting - Discussion Group 1 System Level Design and Development** (Pourmohammadi, Simunovic, Walsh, Ley, *Moderator: Ahmed Eldesoky*)

4:00 - 5:00 pm **Teams Meeting - Discussion Group 2 Sustainability and Green Chemistry** (Martell, Walker, Hale, *Moderator: Tina Taskovic*)

Introductions to Organizations

Representatives of several organizations with an active presence on campus and the community share information about their groups.

Student Energy

Green Chemistry Initiative

Electrochemical Society Student Chapter

Dalhousie Working for Inclusivity in Chemical Sciences

Women in Renewable Energy

The Influence of HF Etching Process on the Photocatalytic H_2 Evolution Reaction Using Mesoporous Si Nanoparticles

Sarah Martell
Department of Chemistry, Dalhousie University

Email: SMartell@dal.ca
Co Authors: Ulrike Werner-Zwanziger, Mita Dasog
Research Supervisor: Prof. Mita Dasog

In this work, the response of the photocatalytic activity of the mpSi nanoparticles to a series of HF acid treatments was investigated.[1] A two-step magnesiothermic reduction method was used to prepare crystalline mpSi nanoparticles with specific surface areas over 500 m^2g^{-1}.[2] In the presence of ≥ 1.0 mL HF per 0.010 g of Si, morphological damage was observed using electron microscopy. N_2 adsorption measurements indicated that the pore size and surface area were also altered. Solution-phase NMR studies indicated the formation of SiF_5^- and SiF_6^{2-} when larger volumes of HF were used. Both factors, morphological damage, and presence of byproducts in the pores, likely result in lowering of the photocatalytic H_2 evolution rate. This study shows that care must be taken when an HF etching step is involved, especially with porous nanoparticles that can trap reaction byproducts.

References

[1] S. A. Martell, U. Werner-Zwanziger, M. Dasog, *Faraday Discuss.* **2020**, 222, 176-189.

[2] S. A. Martell, Y. Lai, E. Traver, J. MacInnis, D. D. Richards, S. MacQuarrie, M. Dasog, *ACS Appl. Nano Mater.* **2019**, 2, 5713 —5719.

Bis(phosphino)silyl Ni Complexes for the Catalytic Hydrogenation of Alkynes

Dylan Hale
Chemistry

Email: dylan.hale@dal.ca
Co Authors: Laura Turculet
Research Supervisor: Prof. Laura Turculet

Catalysts that utilize 3d-metals in lieu of their heavier second and third row congeners have recently attracted significant attention due to the relatively high abundance and low cost of the first row transition metals. While such sustainable catalysts are being utilized for a variety of applications, research in the Turculet group has focused on the catalytic reduction of unsaturated substrates. In this regard, catalysts capable of performing direct alkene and alkyne hydrogenation with H_2 are especially attractive due to the inherent atom economy of this reaction. Previous work in the Turculet group has shown that bis(phosphino)silyl PSiP supported Fe[1] and Co[2] complexes can facilitate alkene hydrogenation through generation of metal hydrides, with the readily isolated complex (PSiP)FeH$(N_2)_2$ proving to be a highly effective, easily manipulated precatalyst for the hydrogenation of a range of terminal and multiply-substituted alkenes. Furthermore, the Turculet group has shown that PSiP supported Ni[3] hydride complexes can perform the selective hydroboration of CO_2 to the formaldehyde level. This presentation focuses on expanding the utility of these Ni hydride complexes to include the catalytic hydrogenation of alkynes under exceptionally mild conditions.

[1] Murphy, L. J.; Ferguson, M. J.; McDonald, R.; Lumsden, M. D.; Turculet, L. *Organometallics* **2018**, 37, 4814-4826.

[2] Murphy, L. J.; Ruddy, A. J.; McDonald, R.; Ferguson, M. J.; Turculet, L. *Eur. J. Inorg. Chem.*, **2018**, 4481-4493.

[3] Murphy, L. J.; Hollenhorst, H.; McDonald, R.; Ferguson, M. J.; Lumsden, M. D.; Turculet, L. *Organometallics* **2017**, 36, 3709-3720.

Evolution of Environmentally Sustainable Wood Preservatives

Kathleen Walker
Engineering

Email: kathleen.walker@dal.ca
Research Supervisor: Dr. Sophia He

Stella-Jones Inc. is a wood preservation cooperation whose focus is the production of pressure treated wood for industrial products. The company is an environmentally responsible enterprise and has been pursuing greener wood treatment processes and minimizing the impact of the manufacturing process on the environment. When the corporation was founded in the 1990's the main wood preservatives used for production included creosote, pentachlorophenol and copper chromium arsenate (CCA). Even though these products produced a high-quality preserved wood, they were harsh on the environment, and had foul odors. To revolutionize the wood preservation industry, Stella-Jones Inc. has been implementing research to make current preservatives environmentally friendlier. In addition to optimizing current preservative blends and operating processes, significant research has been completed to benefit the environment by creating and using safer wood preservative formulations; particularly where environmentally friendlier preservatives have been introduced to the market in recent years. In addition to researching friendlier preservatives, Stella-Jones Inc. has been implementing cleaner technology and researching methods to minimize their environmental impact. These methods range from increased environmental monitoring programs to optimized recycling programs to reduce the quantity of wasted preservative. This talk will highlight the evolution of wood preservatives as well as the future of Stella-Jones' research on evaluation of innovative wood preservative formulations.

The Electronic Properties of Silver Nanoclusters as Determined Through X-ray Absorption Spectroscopy and Density Functional Theory

Andrew Walsh
Chemistry

Email: andrew.walsh@dal.ca
Co Authors: Peng Zhang
Research Supervisor: Prof. Peng Zhang

Atomically precise thiolate-protected silver nanoclusters, containing a countable number of atoms and diameters less than 2 nm,[1] are becoming increasingly studied since they are synthesized in greater yields[2] and show the enhanced catalytic[3] and optical[2] properties observed in other metal nanoclusters. Both density functional theory (DFT) calculations[2] and X-ray absorption spectroscopy (XAS)[4] have been used to examine silver nanoclusters, but the two methods have not yet been combined to fully investigate their electronic properties. This project will employ a joint approach in using both XAS and DFT calculations to analyze the electronic properties of some silver nanoclusters. These results will be correlated to generate a detailed picture of their electronic properties that can help explain other observed properties for these silver nanoclusters.

1. Walsh, A. G.; Chen, Z.; Zhang, P. *J. Phys. Chem. C* **2020**, 124, 4339-4351.

2. Conn, B. E.; Desireddy, A.; Atnagulov, A.; Wickramasinghe, S.; Bhattarai, B.; Yoon, B.; Barnett, R. N.; Abdollahian, Y.; Kim, Y. W.; Griffith, W. P.; Oliver, S. R. J.; Landman, U.; Bigioni, T. P. *J. Phys. Chem. C* **2015**, 119, 11238-11249.

3. Urushizaki, M.; Kitazawa, H.; Takano, S.; Takahata, R.; Yamazoe, S.; Tsukuda, T. *J. Phys. Chem. C* **2015**, 119, 27483-27488.

4. Chevrier, D. M.; Conn, B. E.; Li, B.; Jiang, D.-e.; Bigioni, T. P.; Chatt, A.; Zhang, P. *ACS Nano* **2020**, 14, 8433-8441.

Binder Jet Printing of Low-Cost Tool Steel Powders

Ryan Ley
Mechanical Engineering

Email: Ryan.Ley@dal.ca
Co Authors: Ian Donaldson, Paul Bishop
Research Supervisor: Prof. Paul Bishop

Water atomization is utilized extensively in the high-volume production of iron and steel powders that are destined for use in press-and-sinter powder metallurgy (PM) technology. This particular variant of atomization maintains a low operating cost and typically produces particles that are relatively coarse (D50 ~120 µm) and irregular in shape. While these traits are desirable for PM, they are not necessarily ideal for additive manufacturing (AM). However, with appropriate adjustment of the atomization parameters, a nearly spherical powder with a reduced D50 can be achieved. The objective of this research was to investigate cost-effective, water atomized powders in the context of binder jet printing AM. As such, a water atomized D2 tool steel powder was produced targeting a nominally spherical shape and reduced D50 to aid spreadability and post-print sintering response. The starting powder was characterized in detail using laser light scattering, optical microscopy, SEM, and DSC. Preliminary builds were then printed, de-bound, and vacuum sintered under various conditions in a thermal dilatometer to assess densification behaviour. It was determined that the optimal sintering conditions for maximizing density while still maintaining part geometry was in the range of 1220°C - 1260°C with a hold time of 30 minutes. Secondary testing was then performed to both verify these conditions with larger samples, and to examine the resulting mechanical properties of the sintered products.

A robust simulation-optimization approach for designing hybrid renewable energy systems

Pardis Pourmohammadi
Industrial Engineering

Email: pardis.pourmohammadi@dal.ca
Co Authors: Dr. Ahmed Saif
Research Supervisor: Dr. Ahmed Saif

Stand-alone hybrid renewable energy systems (HRES) provide a viable alternative to satisfy energy demand in remote and isolated communities. We consider a PV/Wind/Diesel/Battery HRES and propose a cost-minimization design approach that uses a finite number of supply and demand scenarios with uncertain probabilities, extracted from limited data through k-means clustering. Using an ambiguity set based on phi-divergence, a novel robust simulation-optimization approach that estimates a surrogate objective function through Response Surface Methodology (RSM) is proposed. Results obtained from implementing the proposed approach on a real case study show that it outperforms classical risk-neutral methods on external data samples.

Laser Scanner for Cell Thickness Mapping and Volume

Zachary Simunovic
Mechanical Engineering

Email: zachary.simunovic@dal.ca
Co Authors: Michael Metzger
Research Supervisor: Prof. Michael Metzger

A precise understanding of the physical properties of lithium-ion cells including cell thickness distribution and its connection with cell lifetime is important for the improvement of cell design. A laser scanning instrument has been developed to perform contact free thickness and volume measurements for lithium-ion cells. Three cell types with different thickness were measured; which included LFP/AG, NMC532/AG, and NMC811/Cu cells. The laser scanning instrument provided thickness values that were lower than the values yielded by a linear gauge which is a conventional method. The linear gauge picks up on elevated features of the pouch cell yielding higher values. Thus, more detailed measurements are needed. The entire surface of a pouch cell can be mapped for thickness using the laser scanner method to further understand the uniformity of a lithium-ion cell, and to calculate its volume.