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MIDWEST REGIONAL CONFERENCE

17th Annual
AIChE Midwest Regional Conference

April 29, 2025

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Organized by the AIChE Chicago Local Section, AIChE Global and the University of Illinois at Chicago

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Conference Overview

The AIChE Midwest Regional Conference (MRC) continues into its 17th year. Organized by the **AIChE Chicago Local Section, AIChE Global** and the **University of Illinois at Chicago**, the MRC provides an opportunity for engineers and scientists in the region to learn about new technologies and network with others in the field. A particular objective of the conference is to build technical relationships between industrial practitioners and researchers in the governmental and academic spheres. The technical program includes:

3 Keynote Lectures:

- **Professor Y. Shirley Meng,** *Professor at the Pritzker School of Molecular Engineering at the University of Chicago*
- **Dr. Zara Summers,** *Chief Science Officer at LanzaTech*
- **Professor David E. Bernal Neira,** *Assistant Professor at the Davidson School of Chemical Engineering at Purdue University*

The conference contains **12 technical sessions** featuring over **40 oral presentations.** The evening portion is combined with the **AIChE Chicago Local Section Monthly Meeting**.

On behalf of the conference planning committee, we welcome you to the 17th Annual AIChE Midwest Regional Conference and hope you will take advantage of all the opportunities it has to offer.

Jarad Champion
Conference Chair
Geosyntec

Jason Wu
Program Chair
Honeywell UOP

Gengnan Li
Program Co-Chair
Argonne National Laboratory

Program at a Glance

Tuesday, April 29th, 2025

7:00 – 8:00 AM **Registration and Breakfast** (Fort Dearborn Room)

8:00 – 8:15 AM **Conference Introduction** (Illinois Room B)

8:15 – 9:45 AM **Session I**

Track 1	**Track 2**	**Track 3**
Fluids (White Oak)	Polymers & Materials (Illinois Room C)	Process Safety (Cardinal Room)

9:45 – 10:00 AM **Break**

10:00 – 11:00 AM **1st Morning Keynote** (Cardinal Room)
Dr. Zara Summers, *LanzaTech,*
Bridging Biology and Engineering: Pioneering Sustainable Solutions through Carbon Recycling

11:00 – 11:10 AM **Break**

11:10 – 12:00 PM **Session II**

Track 1	**Track 2**	**Track 3**
Catalysis I (White Oak)	Career Development (Illinois Room C)	Circularity/Sustainability I (Cardinal Room)

12:00 – 1:00 PM **Lunch** (Illinois Room B)

1:00 – 2:00 PM **2nd Afternoon Keynote** (Cardinal Room)
Prof. Shirley Meng, *UChicago, Argonne National Lab*
Global Race for A Better Battery

2:00 – 2:10 PM **Break**

2:10 – 3:20 PM **Session III**

Track 1	**Track 2**	**Track 3**
Catalysis II (White Oak)	Bio-Engineering (Illinois Room C)	Circularity/Sustainability II (Cardinal Room)

3:20 – 3:25 PM **Break**

3:25 – 4:45 PM **Session IV**

Track 1	**Track 2**	**Track 3**
Catalysis III (White Oak)	Process Systems (Illinois Room C)	Energy Storage (Cardinal Room)

4:30 – 5:45 PM **Poster Session** (Illinois Room A)

5:45 – 7:30 PM **Chicago Section Dinner** (Illinois Room B)
Dinner Keynote – Prof. David Neira, *Purdue University*
Perspectives of Quantum Computing in Chemical Engineering

Keynote Speakers

Tuesday Morning Keynote, 10:00 AM – 11:00 AM

Dr. Zara Summers, *Chief Science Officer, LanzaTech*

Dr. Zara Summers is the Chief Science Officer at LanzaTech, where she leads a team of over 200 scientists dedicated to transforming waste carbon into sustainable fuels, chemicals, materials, and protein for everyday products. Before joining LanzaTech in January 2022, Dr. Summers held a pivotal role at ExxonMobil, where she spearheaded the creation of their R&D Bioscience division and managed a comprehensive portfolio of bio-based programs, including strategies for nature-based solutions.

Dr. Summers' expertise lies in the field of biology and engineering, with a particular focus on sustainability and environmental research. Her work at LanzaTech revolves around pioneering novel biorecycling technologies that capture carbon emissions from energy-intensive industries, repurposing them into valuable products that replace virgin fossil carbon. Her innovative approach has been instrumental in advancing a circular carbon economy through strategic partnerships with companies such as ArcelorMittal, Zara, H&M Move, Coty, On, and LanzaJet.

A recipient of numerous honors and awards, Dr. Summers is recognized as a leading expert in her field. She holds a Ph.D. in Microbiology, which underpins her scientific and technical contributions to sustainable solutions. Her extensive professional experience includes leadership roles in matrixed organizations, complex problem-solving through fundamental science, and scaling up technology. Additionally, she excels in communication and partnership development, collaborating with industry groups, professional societies, NGOs, and global research institutions.

At LanzaTech, Dr. Summers oversees the Science division, including Synthetic Biology, Fermentation, Global Services, and the Freedom Pines, GA division. She is accountable for the company's technology pipeline and technical portfolio, regularly briefing the Board of Directors on scientific advancements and strategic direction. Recently, her team expanded LanzaTech's biorefining platform to produce commercial-scale nutritional protein from CO_2, addressing food security concerns with a cost-competitive, resource-efficient solution.

Throughout her career, Dr. Summers has been a devoted advocate for using biology to combat climate change and has been a champion for women in STEM. She strives to create opportunities for all and push forward the commercialization of decarbonization technologies to ensure a sustainable future for humanity.

Tuesday Afternoon Keynote, 1:00 – 2:00 PM

Prof. Y. Shirley Meng, Professor at the *Pritzker School of Molecular Engineering, University of Chicago*

Dr. Y. Shirley Meng serves as the Chief Scientist of the Argonne Collaborative Center for Energy Storage Science (ACCESS) Argonne National Laboratory. Dr. Meng is the director of **Energy Storage Research Alliance (ESRA),** an innovation hub funded by US Department of Energy, Office of Science.

She is the principal investigator of the research group - **Laboratory for Energy Storage and Conversion (LESC),** that was established at University of California San Diego since 2009. She held the Zable Chair Professor in Energy Technologies at UC San Diego from 2017-2022 and founded the **Sustainable Power and Energy Center (SPEC)** in 2016. Dr. Meng received several prestigious awards, including ACS Research Excellence in Electrochemistry (2024), ECS Battery Division Research Award (2023), the C3E technology and innovation award (2022), the Faraday Medal of Royal Chemistry Society (2020), International Battery Association IBA Research Award (2019), Blavatnik Awards for Young Scientists Finalist (2018), C.W. Tobias Young Investigator Award of the Electrochemical Society (2016) and NSF CAREER Award (2011). Dr. Meng is elected Fellow *of Electrochemical Society (FECS), Fellow of Materials Research Society (FMRS) and Fellow of American Association for the Advancement of Science (AAAS).* She is the author and co-author of more than 320 peer-reviewed journal articles, two book chapters and twelve issued patents. Dr. Meng received her Ph.D. in Advance Materials for Micro & Nano Systems from the *Singapore-MIT Alliance* in 2005. She received her bachelor's degree in Materials Science with first class honor from Nanyang Technological University of Singapore in 2000.

Tuesday Evening Keynote, 6:30 – 7:30 PM

Prof. David E. Bernal Neira, *Assistant Professor, Davidson School of Chemical Engineering , Purdue University*

David E. Bernal Neira specializes in applying mathematical and computer science tools to address problems relevant to science and engineering, for example, physics and chemical, process, and energy systems engineering. In particular, he works in nonlinear discrete optimization, where, besides applications, he has been working in theory, algorithms, and software. He has been involved in research and teaching related to these topics for over a decade, complemented with research in Quantum Computing. He is a member of the Purdue Quantum Science and Egnineering Institute (PQSEI) and the Chicago Quantum Exchange.

Program

8:00 – 8:15 AM **Conference Introduction**

8:15 – 9:45 AM **Session 1**

Track 1
Fluids

8:15 – 8:40 AM
Interfacial Separations By a Polydimethylsiloxane (PDMS)Layer. Molecular Modeling of Coated Stir Bar Extraction of Organics from Aqueous Solutions, Abdulazez Alzhrani, *Illinois Institute of Technology*

8:40 – 9:05 AM
Optimization of Reverse-Osmosis MD Simulations Using Molecular Replication, Bandar Bashmmakh, *Illinois Institute of Technology*

9:05 – 9:25 AM
Mass Transfer in Mini-Hollow Fiber Membrane Solvent Extraction for Biobutanol Recovery,
Thanh Tin Nguyen, *Argonne National Laboratory*

9:25 – 9:45 AM
Novel Analysis Methods for Dense Frictional Suspension Rheology: Expanding Granular Mechanics Analysis Methods for Dense Suspensions, Alessandro d'Amico, *Case Western Reserve University*

Track 2
Polymers & New Materials

8:15 – 8:40 AM
Effects of Lignin Structure on the Performance of Cellulose-Lignin Biodegradable Films, Taiwo Adesanya,
University of Illinois Chicago

8:40 – 8:55 AM
Green Synthesis of Gold Nanoparticles Using American Ginseng, Sonia Grade, *Milwaukee School of Engineering*

8:55 – 9:20 AM
Development of Poly(Isatin Fluorene) with Tert-Butyloxycarbonyl (BOC) Group for Organic Solvent Nanofiltration Membranes, Chaoyi Ba, *Argonne National Laboratory*

9:20 – 9:45 AM
A Platform of Iron and Gold Nanoparticles for Biosensing Applications, Aakash Gupta, Weizheng Wang,
University of Wisconsin Milwaukee

Track 3
Process Safety

8:15 – 8:40 AM
NFPA 660 and a Dust Hazard Analysis Case Study, Katie Kuhn, *Fauske and Associates*

8:40 – 9:05 AM
Sulfur Pit Safety – The Black Sheep of Process Safety, Eleftherios Avtzis, *Brindley Engineering*

9:05 – 9:25 AM
Combustible Dust Testing: What Testing Can Tell You about Your Facility's Dust Hazards, Danielle Kittaka, *Fauske and Associates*

9:25 – 9:45 AM
Hazards and Fundamentals of Handling and Transferring Flammable, Caustic, and Toxic Liquid Chemicals in Non-Steady-State Operations, Trevor Lardinois, *Exponent Inc*

9:45 – 10:00 AM **Break**

10:00 – 11:00 AM **1st Keynote Speaker:**
Dr. Zara Summers, *Lanza Tech*
Bridging Biology and Engineering: Pioneering Sustainable Solutions through Carbon Recycling

11:00 – 11:10 AM **Break**

11:10 AM– 12:00 PM **Session 2**

Track 1
Catalysis I

11:10 – 11:20 AM
Mixtures of Ionic Liquids and Deep Eutectic Solvents for Accelerating Reactive Carbon Capture, Bianca Berry, *Lyons Township High School*

11:20 – 11:40 AM
Sustainable Oxalate Production Via Nonaqueous Electrochemical CO2 Reduction Using Earth-Abundant Iron Catalysts, Rohan Sartape, *University of Illinois Chicago*

11:40 – 12:00 PM
Isomerization of Epoxides By Tris(Pentafluorophenyl)Borane (BCF): Investigation of Solvent Effects,
Hiyab Mekonnen, *Northwestern University*

Track 2
Career Development

11:10 – 11:35 AM
Important Data for Your Project Sponsor Relationship, Annette A. Johnston, *AAJ Project Consulting LLC*

11:35 – 12:00 PM
Compensation Trends and the Job Market for Chemical Engineers, Adam Krueger, *Sun Recruiting*

Track 3
Circularity & Sustainability I

11:10 – 11:35 AM
Analysis of the Environmental Impacts and Plausible Recyclability Effects of Additives in Plastics,
Pahola Thathiana Benavides, *Argonne National Laboratory*

11:35 – 12:00 PM
Plasma-Assisted Low Temperature Low Pressure CO2 Conversion to E-Fuels, Ghassan Alshehry, *Saudi Aramco PE&D EXPEC ARC*

12:00 – 1:00 PM **Lunch**

1:00 – 2:00 PM **2nd Keynote Speaker:**
Prof. Y. Shirley Meng, *University of Chicago*
Global Race for A Better Battery

2:00 – 2:10 PM **Break**

2:10 – 3:20 PM **Session 3**

Track 1
Catalysis II

2:10 – 2:35 PM
Exploring the Influence of Low Pt Loadings on Overlayered Mo-Nitrides for Selective Hydrogenation, Siobhan Brown, *Northwestern University*

2:35 – 3:00 PM
Competitive Valerate Binding Enables RuO2-Mediated Butene Electrosynthesis in Water, Špela Kunstelj, *University of Chicago*

3:00 – 3:20 PM
In Situ Kinetic Analysis of Plasma-Enhanced Strong Metal-Support Interactions, Russell J. Clarke, *University of Notre Dame*

Track 2
Bio-engineering

2:10 – 2:35 PM
Recovery of Organic Acids from Processed Biomass Using Advanced Ionomers and Electrochemical Separations, Christopher Arges, *Pennsylvania State University*

2:35 – 3:00 PM
Life-Cycle Analysis of Microalgae-Based Polyurethane Foams, Ulises R. Gracida-Alvarez

3:00 – 3:20 PM
Mitigating Bioaerosol Risks from Industrial Cooling and Wastewater Systems, William Celenza, *Burns & McDonnell*

Track 3
Circularity & Sustainability II

2:10 – 2:35 PM
Dynamic Simulation of CO_2 Adsorption in Amine-Based Sorbents for Direct Air Capture, Dana Marinic, *National Institute of Chemistry*

2:35 – 3:00 PM
A Techno-Economic Analysis of Virgin Lithium Compounds Production from Conventional Pathways, Sabine Gallagher, *Argonne National Laboratory*

3:00 – 3:20 PM
Poly(3-hydroxybutyrate)-Laminated Trilayer Composite Film for Active Food Packaging Application, Shu Xu, *Argonne National Laboratory*

3:20 – 3:25 PM Break

3:25 – 4:45 PM Session 4

Track 1
Catalysis III

3:25 – 3:50 PM
Tandem CO2-Oxidative Propane Dehydrogenation By in2O3-Overcoated Pt Catalyst, Geunho Han, *Northwestern University*

3:50 – 4:15 PM
Molybdenum Nitride on Platinum-Alumina for Ammonia Synthesis, Vinita Dubey, *Northwestern University*

4:15 – 4:40 PM
Ethylene and Propylene Co-Oligomerization in Mesoporous Catalysts, Alba Scotto d'Apollonia, *University of Notre Dame*

Track 2
Process Systems / AI/ML

3:25 – 3:45 PM
Process Modeling and Techno-Economic Optimization for Production of Lignin-Isolated Soy Protein-Based Bio-Adhesive, Poulomi Das, *West Virginia University*

3:45 – 4:05 PM
Computational Optimization and Machine Learning Modeling of Membrane-Assisted Bio-Methanol Dehydration, Hamta Bardool, *Purdue University*

4:05 – 4:25 PM
Introducing a Bayesian Approach for Sparse Modeling of Time-Delayed Process Systems, Samuel Adeyemo, *Calvin University*

4:25 – 4:45 PM
Development of an Online Health Monitoring Framework for High-Temperature Boiler Components by Using Hybrid First Principles-Artificial Intelligence Models, Vivek Saini, *West Virginia University*

Track 3
57801 Energy Storage

3:25 – 3:50 PM
Cost Modeling of Cathode Active Materials in Electric Vehicle Batteries, Kevin Knehr, *Argonne National Laboratory*

3:50 – 4:15 PM
Powering the Future: Challenges and Opportunities in Electrical Generation, Maria Salazar, *Chemistry in Business and Education*

4:15 – 4:40 PM
Impact of Thermal Gradients on the Dynamics of Cylindrical Lithium-Ion Cells and the Module Performance, Mohammed Effat, *Argonne National Laboratory*

4:30 – 5:45 PM **Poster Session**

5:45 – 7:30 PM **Dinner**
3rd **Keynote Speaker:**
Prof. David E. Bernal Neira, *Purdue University*
Perspectives of Quantum Computing in Chemical Engineering

Presentation Abstracts

Session 1

Track 1
Fluids

Chair: Jason Wu

Interfacial Separations by a Polydimethylsiloxane (PDMS)Layer. Molecular Modeling of Coated Stir Bar Extraction of Organics from Aqueous Solutions

Abdulazez Alzhrani, Sohail Murad, *Illinois Institute of Technology*, Cynthia J. Jameson, *University of Illinois at Chicago*

Separation processes relying on interfacial interactions, such as the Stir Bar Sorptive Extraction represent one of the most critical methods of analyte trace organic detection and extraction in environmental, food, and biomedical samples. While the use of polydimethylsiloxane (PDMS) as a sorptive coating in SBSE has exhibited high sensitivity and efficiency; the molecular mechanisms involved are less explored. We report molecular simulation studies using Molecular Dynamics (MD) to investigate the absorption of organic compounds including phenol, chlorophenol, guaiacol, benzyl alcohol, and phenethyl alcohol at the aqueous-PDMS interface, and focus on temperature-dependent behavior. By employing an appropriate force field for PDMS, organic compounds, and water, these simulations directly predict PDMS-Water partition coefficients, diffusion coefficients, and solubilities in the PDMS phase without relying on octanol-water partitioning as a surrogate. An important result of the MD simulations in this work is our ability to predict the temperature dependence of the log p(PDMS/water). Results reveal a non-monotonic temperature-dependent sorption trend for log P [PDMS/water] values. However, we find that with increasing temperature, the absolute number of organic molecules in the PDMS phase increases, driven by enhanced molecular diffusion and PDMS's significant sorption capacity. The findings demonstrate that performing SBSE at elevated temperatures can enhance analyte uptake, improving the analytical sensitivity of trace level extractions, where achieving sufficient analyte concentration in the sorptive phase is critical for reliable detection and quantification in a wide variety of applications in environmental monitoring.These simulations demonstrate that temperature is key to optimizing SBSE and MD captures its molecular interactions.

Optimization of Reverse-Osmosis MD Simulations Using Molecular Replication

Bandar Bashmmakh, Sohail Murad, *Illinois Institute of Technology*, Kevin Hinkle, *University of Dayton*, Cynthia J. Jameson, *University of Illinois at Chicago*

Studies of membrane-based reverse-osmosis systems using molecular dynamics have been widely conducted with accessible computational facilities. However, the study of extremely diluted solutions using molecular dynamics is extremely rare due to the high computational cost associated with having a very large number of particles in the system. Using our new approach, we extend the study of reverse-osmosis system in molecular dynamics simulations to extremely dilute solutions, i.e. ppm solute concentrations through the molecular replication. Through the new approach, we observed a significant computational time saving where the new system achieves almost identical results 41 times faster than the traditional method used in such studies. Properties used for comparison between the two approaches include: (i) density profiles of solvent and solute particles along the permeation direction, (ii) solute-solvent, solvent-solvent, and solute-solute RDFs and ADFs, (iii) solute particles coordination numbers, and (iv) solute particles solvation energies. Our molecular-replication reverse-osmosis method can be applied to porous membranes materials. In this demonstration, we show the effectiveness of the method by concentrating a dilute LiCl using two membranes: a semi-permeable FCC membrane that was used in benchmarking the new method in addition to a hydrophobic Silicalite (MFI type) zeolite which has been proposed for use in water treatment.

Mass Transfer in Mini-Hollow Fiber Membrane Solvent Extraction for Biobutanol Recovery

Thanh Tin Nguyen, Lauren Valentino, Meltem Urgun-Demirtas , *Argonne National Laboratory*

Membrane solvent extraction (MSE) is emerging as a promising technology for resource recovery thanks to its ability to enhance mass transfer between immiscible liquid phases without direct interaction. Extracting biobutanol from fermentation broths poses difficulties because of its low concentration and the existence of inhibitory substances. MSE offers a promising solution by enabling selective extraction with minimal energy consumption. This study initially evaluates the effects of trans-membrane pressure (ΔP = 5–11 psi) and aqueous flow rates (20–50 mL/min) on biobutanol recovery utilizing a hollow fiber membrane contactor. A mini-module with a membrane area of 24 cm^2 was designed, with the organic phase flowing through the lumen and the aqueous phase on the shell side. Experimental results, devoid of fouling effects, indicated that a trans-membrane pressure of 9 psi effectively mitigates organic/water crossover and prevents pressure buildup in the lumen arising from emulsion formation. Higher aqueous flow rates enhance mass transfer, improving biobutanol recovery. A resistance-in-series model will be employed to analyze the mass transfer in the mini modules comprehensively. The presentation will discuss and validate the local mass transfer coefficients and fractional resistances. Our upcoming work will introduce in-situ imaging techniques, i.e., direct fouling observation on mini-hollow fiber membrane modules, facilitating a comprehensive analysis of the fouling mechanism. Notably, mini-modules are advantageous for their cost-effectiveness, reduced sample volume, and suitability for fouling analysis. The initial findings will support the development of an advanced model that incorporates fouling effects in MSE for efficient biobutanol recovery from fermentation broths.

Novel Analysis Methods for Dense Frictional Suspension Rheology: Expanding Granular Mechanics Analysis Methods for Dense Suspensions.

Alessandro d'Amico, Sidong Tu and Abhinendra Singh, *Case Western Reserve University*

Dense suspensions exhibit strongly non-Newtonian behavior under shear with strong increases in viscosity called shear thickening. With sufficient stress, the suspension's interparticle interactions transitions from predominantly lubricated to frictional-contact-forces dominated state. Frictional contacts between particles stabilize the contact network thus providing resistance to external deformation. This interparticle frictional contact network drives shear thickening but its characterisation remains elusive. We use a cycle characterization technique to analyze the frictional contact network in the dynamic steady state. We find that the third-order loops within the frictional contact network is the main driver of the viscosity and can help us to predict the suspension viscosity regardless of packing fraction, applied external stress, interparticle friction coefficient. This study further elucidates the crucial role of the mesoscale network in connecting the microscopic physics to the macroscopic bulk response of the material. We can characterize our network and collapse the high dimensionality of the microscopic-to-macroscopic phase diagram. As a result, network analysis can now predict system viscosity regardless of stress, interparticle coefficient of friction, and packing fraction. This further elucidates that unweighted mesoscopic network topology determines system viscosity.

Track 2
Polymers & New Materials

Chair: Wujie Zhang

Effects of Lignin Structure on the Performance of Cellulose-Lignin Biodegradable Films

Taiwo Adesanya, Ezinne Achinivu-Ibagere, *University of Illinois Chicago*

The development of high-performing biobased packaging material as a potential replacement for low-

density polyethylene (LDPE) can combat the plastic pollution problem. The experimental and computational evaluation of protic (PIL) and aprotic ionic liquid (AIL)-cosolvent system for dissolution and blending of cellulose, a structural polymer, and lignin, a barrier matrix, to fabricate bioplastics are reported. Thereafter, extensive characterization and benchmarking with LDPE and Biobag, a commercial bioplastic, were conducted to ensure adequate strength, processability, appeal to users, protection of the packaged product from environmental factors (water vapor, UV-rays, and oxidants), and biodegradation. These cellulose-lignin films demonstrated superior UV-blocking, faster biodegradation, and lower thermal degradation temperatures. They exhibit comparable surface roughness with LDPE. 100% cellulose had a comparable water vapor transmission rate (WVTR) with the Biobag. The plasticizing and barrier effects of hardwood, softwood, grasses, and technical lignin were evaluated to reduce brittleness and water vapor transmission rates. The percentage elongation at break ($\%E_b$) varies with lignin source structure following the trend: Grassy lignin increased $\%E_b$, softwood lignin reduced $\%E_b$ while technical & hardwood lignin had a near neutral effect on $\%E_b$. WVTR depends on lignin monomers' total polar surface area (tPSA), which drives the affinity for water vapor. Antioxidant properties depend on both pKa and bond dissociation energy (BDE) of monomer's phenolic hydroxyl groups. These results show that cellulose & lignin, abundant biobased materials, can be processed with environmentally friendly methods to yield bioplastic with improved protective capacity for packaged products while demonstrating comparable mechanical capacity & smoothness as LDPE.

Green Synthesis of Gold Nanoparticles Using American Ginseng

Sonia Grade, Emma Klatt, Ben Lilienkamp, Milwaukee School of Engineering

Gold nanoparticles (Au NPs) have been extensively utilized in biomedical fields, such as drug delivery and medical imaging. The focus of this study was the green synthesis of gold nanoparticles using American ginseng (Panax quinquefolium). Extracts of the American ginseng's roots, stems, and leaves were compared, the results indicated that the extract of leaves exhibiting the the highest efficiency in Au NP synthesis and, thus, were used in the Au NP synthesis. The green synthesized Au NPs were characterized using scanning electron microscopy-energy-dispersive X-ray spectroscopy (SEM-EDX) and attenuated total reflection Fourier transform infrared spectroscopy (ATR-FTIR). The Au NPs were spherically shaped with a diameter of 18 nm and uniform distribution throughout as well as a characteristic absorbance peak at ~529 nm. HeLa cells were utilized in a cytotoxicity study that showed the inhibition of cell proliferation but the cell viability remained constant (>99%). Overall, the Au NPs synthesize using the extract of American ginseng leaves show great potential in various biomedical applications.

Development of Poly(Isatin Fluorene) with Tert-Butyloxycarbonyl (BOC) Group for Organic Solvent Nanofiltration Membranes

Chaoyi Ba, Shu Xu, Vivek Adepu, Lauren Valentino, Meltem Urgun-Demirtas, *Argonne National Laboratory*

Organic solvent nanofiltration (OSN) membranes offer a lower-energy, scalable, and intensified alternative to traditional thermal separation processes, reducing both costs and greenhouse gas (GHG) emissions. Despite their potential, the widespread adoption of OSN membranes at large scale is hindered by challenges such as the permeability-selectivity trade-off, and limited resistance to extreme conditions (e.g., high temperatures, corrosive or acidic environments, or mixed streams with plasticizing agents). In this work, we present a novel polymer, poly(isatin fluorene) with a ***tert***-butyloxycarbonyl (BOC) group grafted to the isatin unit (PIF-Boc). This polymer exhibits excellent solubility in chloroform, enabling efficient processing for the fabrication of thin-film composite (TFC) membranes. Commercial polyacrylonitrile (PAN) membranes were coated with a thin PIF-Boc selective layer, resulting in a shiny, smooth, and uniform surface. FTIR analysis confirmed the successful lamination of the barrier layer, as evidenced by the characteristic three carbonyl peaks of PIF-Boc. The resulting TFC membranes demonstrated separation performance (e.g., permeance and selectivity) comparable to commercial silicone-based OSN membranes while achieving cost savings of over threefold. These findings highlight the potential of PIF-

Boc as a cost-effective material for advanced OSN membrane applications.

A Platform of Iron and Gold Nanoparticles for Biosensing Applications

Aakash Gupta, Weizheng Wang, Qingsu Cheng,
University of Wisconsin Milwaukee

Nanoparticles (NPs) have garnered significant interest as a platform for biosensing applications, including medical diagnostics, environmental monitoring, food safety, biodefense, and pharmaceutical research. Because of the unique physical, chemical, and optical properties carried by NPs, using them would enhance selectivity and sensitivity. Here, we report the fabrication of magnetic ferric oxide (Fe_3O_4-COOH NPs) and gold nanoparticles (Au NPs) with proteins and aptamers, respectively. The Fe_3O_4-COOH NPs were functionalized with BSA-FITC via a cross-linking reaction between the carboxylic acid groups on the functionalized nanoparticles and the available amine (NH_2) groups on the BSA-FITC protein. Similarly, the Au NPs were conjugated with aptamers by covalent binding between the Au NPs and the aptamers containing sulfhydryl functional groups. The success of the conjugation of BSA-FITC molecules on the surface of the functionalized Fe NPs and aptamers on the surface of Au NPs was characterized using UV-Vis, Fluorescence, Fourier-transform infrared (FTIR) spectroscopy and Raman spectroscopy. This approach demonstrates the potential fabrication method for rapid and selective biosensing. With its simplicity, cost-effectiveness, and high sensitivity and selectivity, these NP-based biosensing system presents a promising tool for biomedical applications and public health surveillance.

Track 3
Process Safety

Chair: Jessica Morris

NFPA 660 and a Dust Hazard Analysis Case Study

Katie Kuhn, Danielle Kittaka, *Fauske and Associates*

This presentation will first discuss the release of NFPA 660, the newest standard for combustible dusts and particulate solids. The consolidation of the prior NFPA combustible dust standards will be addressed, as well as the regulatory impacts of the new standard. In addition, a DHA case study will be presented which covers a wood dust deflagration event that occurred in a wood pellet manufacturing plant. The presentation will dive into the root causes of the event and its effects, which includes the material characteristics, the plants processing operations, the safeguards that were in place, and the safety gaps that existed.

Combustible dust exists in numerous industries, including food, grain, plastics, rubber, pharmaceuticals, coal, metals, paper, etc. They are a recognized hazard which can manifest in a variety of different ways. While each industrial environment containing combustible dusts is unique and presents its own specific hazards, principles of inherently safer design and the inherent nature of combustible dusts can be understood. A risk assessment is required to thoroughly and adequately address the hazards presented by combustible dusts on a case-by-case basis. NFPA 660 consolidates and clarifies the best engineering practices to be applied when working with combustible dusts in an industrial setting.

The case study provided insight into several factors which either led to, or exacerbated the initial combustible dust event. This includes: the impact of changing material characteristics within a facility, ignition source control, and properly designed deflagration venting.

Sulfur Pit Safety – the Black Sheep of Process Safety

Eleftherios Avtzis, *Brindley Engineering*

Sulfur Pits are ubiquitous within the petroleum refining industry. Sulfur must be removed from refined liquid products in order to meet regulations via the Claus Sulfur Recovery Unit, where gaseous Sulfur compounds are converted to elemental Sulfur. The elemental Sulfur, within a narrow temperature range, is then stored within Sulfur Pits as molten Sulfur.

NFPA 655 provides guidance on mitigating sulfur pit fires by limiting the concentration of Hydrogen Sulfide (H_2S) in the vapor space and shutting down at a given

threshold. However, there is little in the way of Recognized and Generally Accepted Good Engineering Practices (RAGAGEP) when it comes to monitoring H_2S within and around the Sulfur Pit nor what a shutdown of the pit entails.

Many of the refinery operated Sulfur Pits within the United States of America are now operating beyond their design life and are in need of restoration. Retrofitting a Sulfur Pit presents an opportunity to enhance the safety measures. This presentation will explore various methods for controlling the vapor space of a Sulfur Pit as well as other aspects for Sulfur Pit safety, such as appropriate metallurgy, snuffing steam system design basics, and static discharge mitigation.

Combustible Dust Testing: What Testing Can Tell You about Your Facility's Dust Hazards

Danielle Kittaka, Katie Kuhn, *Fauske and Associates*

This presentation will discuss how combustible dust testing can identify various hazards present in dust-handling facilities. Combustible dust can present fire, flash fire, and explosion hazards, depending on the conditions. It is important to know if dust is combustible in a pile, in cloud form, or both. Dust testing reveals what hazards could occur and what protective measures are effective. Knowing a dust's characteristics can allows one to determine the precautions that should be taken in handling, processing and storing combustible dusts. Some dusts may be sensitive to common ignition sources like static electricity or hot surfaces, and precautions should be taken to reduce chance of ignition. Dust tests have been developed by entities like ASTM, ISO, IEC, VDI and CEN/CENELEC to enable data to be consistent and comparable. Hazard Identification is the first step in a Dust Hazard Analysis as defined by NFPA 660: Standard for Combustible Dusts and Particulate Solids. This standard requires that a facility processing or handling combustible dust performs a hazard analysis for each affected operation.

Hazards and Fundamentals of Handling and Transferring Flammable, Caustic, and Toxic Liquid Chemicals in Non-Steady-State Operations

Trevor Lardinois, Emily Schroeder, Delmar Morrison, *Exponent, Inc.*

Steady-state chemical processing of flammable, caustic, and toxic liquids creates hazards and risks which are identified and managed via process safety. However, in some instances, unsteady-state or batch-wise transfers of hazardous chemicals, such as filling of supply tanks, have not received the same level of process safety oversight at chemical facilities, especially when they are infrequent or ad hoc in nature. The resulting gaps in process safety management, such as a lack of engineering controls, job hazard analysis, or proper personnel training, have resulted in incidents that have injured workers, caused fires or explosions, and polluted the environment. This presentation will provide a variety of case studies related to incidents involving unsteady-state or batch-wise transfers of hazardous chemicals. In addition to identifying the gaps in process safety management, we will explore the fundamentals of the incidents, such as electrostatic ignition of flammable vapors, unanticipated fluid dynamics, and technological challenges with environmental remediation. Attendees will gain valuable insights into identifying hazards and improving process safety management for unsteady-state operations, ultimately safeguarding workers, facilities, and environment.

Morning Keynote

Bridging Biology and Engineering: Pioneering Sustainable Solutions through Carbon Recycling

Zara Summers, LanzaTech

In this keynote , Zara will delve into the current state of the carbon recycling and synthetic biology industries, showcasing innovative technologies driving sustainable solutions. Highlighting LanzaTech's role in transforming waste carbon into valuable raw materials, Zara illustrates the power of biomanufacturing in creating eco-friendly alternatives to traditional manufacturing.

Specifically, Zara will elaborate on LanzaTech's gas fermentation technology. By utilizing proprietary microbes, LanzaTech captures waste gases from industrial sources—such as steel mills, refineries, and landfills—and converts them into ethanol and other valuable chemicals. This innovative process not only reduces greenhouse gas emissions but also provides a sustainable alternative to fossil-derived products. Zara will discuss the successful implementation of this technology in various global facilities, demonstrating the scalability and versatility of LanzaTech's approach. The future holds a vast array of solutions for carbon reduction. She will emphasize the incredible potential of marrying biology and engineering, which offers new opportunities to innovate and produce sustainable outcomes. By integrating these disciplines, we can develop advanced bioengineering techniques that not only mitigate carbon emissions but also create new pathways for renewable energy, sustainable agriculture, and green manufacturing.

Sharing her professional journey, Zara offers insights into the challenges and achievements in her field, providing valuable lessons for students aspiring to contribute to scientific discovery. Her story exemplifies the fusion of biology and engineering and showcases the transformative impact of interdisciplinary collaboration on our ability to combat climate change.

Session 2

Track 1
Catalysis I

Chair: Trevor Lardinois
Co-Chair: Soroush Almassi

Mixtures of Ionic Liquids and Deep Eutectic Solvents for Accelerating Reactive Carbon Capture

Bianca Berry, *Lyons Township High School*, Rohan Sartape, Vamsi Vikram Gande, Sophia Johnson, Meenesh Singh, *University of Illinois Chicago*, Amey Thorat, Rashmi Mishra, *Oklahoma State University*

Industrial CO_2 emissions drive climate change, necessitating energy intensive and chemically robust capture technologies. Deep eutectic solvents (DES) and ionic liquids (ILs)—and their mixtures (DES-IL)— are promising media for CO_2 sequestration due to their low volatility and tunable properties. In this study, we use an automated conductometric platform (sample volume <500 µL) to monitor CO_2 chemisorption in dilute mixtures with N_2. We observed up to a six-fold rate enhancement in DES-IL mixtures compared to DES alone, with all kinetics following a pseudo-first-order model (R^2>0.9). Notably, increasing IL alkyl chain length boosts the capture rate, whereas excessive IL concentration reduces it. Nuclear magnetic resonance spectra and thermodynamic (Arrhenius and Eyring) analyses indicate that free IL cations stabilize the transition state in the nucleophilic addition reaction, providing a plausible mechanistic explanation. These findings advance the design of DES-IL systems for more efficient industrial CO_2 capture.

Sustainable Oxalate Production Via Nonaqueous Electrochemical CO_2 Reduction Using Earth-Abundant Iron Catalysts

Rohan Sartape, Rohit Chauhan, Vamsi Vikram Gande, Ishita Goyal, Yancun Qi, Meenesh R Singh, *University of Illinois Chicago*

Electrochemical CO_2 reduction (eCO2R) is emerging as an attractive technology to address global boiling and convert CO_2 into value-added chemicals. Nonaqueous eCO2R, in particular, offers a promising alternative to aqueous systems by readily producing commercially profitable oxalates. In this study, we report the use of iron (Fe) as an electrocatalyst, achieving a Faradaic efficiency of up to ~75% toward oxalate formation and an overall current density of 25 mA/cm^2. The employment of Fe not only demonstrates high catalytic performance but also provides a safer and more sustainable alternative to toxic catalysts such as Pb that dominate the nonaqueous eCO2R literature. To gain deeper insight into the reaction mechanism, we utilized ATR-SEIRAS to investigate the adsorbed surface intermediates, thereby elucidating a detailed reaction pathway for oxalate synthesis. These findings pave the way for further optimization and scale-up of the process, offering a viable route for sustainable chemical production and CO_2 mitigation.

Isomerization of Epoxides By Tris(Pentafluorophenyl)Borane (BCF): Investigation of Solvent Effects

Hiyab Mekonnen, Guanhua Wang, Justin Notestein, *Northwestern University*

Epoxides are valuable intermediates in organic synthesis, enabling the production of key building blocks such as aldehydes, ketones, and alcohols. Among these transformations, the Meinwald rearrangement offers a direct route to aldehydes or ketones, where regioselectivity is critical for obtaining the desired carbonyl product. The regioselectivity is primarily governed by the migratory aptitude of the epoxide substituents, the catalyst employed and the solvent environment.

Here, we report tris(pentaflurophenyl)borane (BCF) as a Lewis acid catalyst for the Meinwald rearrangement, using propylene oxide (PO) as a model substrate. We systematically examine the effects of water concentration, temperature, and solvent properties such as — coordination strength, polarity, and hydrogen bonding — on BCF's catalytic activity, reaction rates, and product distribution. Then we apply these observations to other epoxide substrates and related arylborane catalysts.

Our findings show that BCF can be very active for the Meinwald rearrangement to aldehydes and that hydrogen bonding solvents suppress other side reactions such as hydrolysis by residual water and the formation of linear or cyclic oligomers. Additionally, in the presence of strongly coordinating solvents like diglyme and proglyde, a rate-acceleratory behavior characterized by an activation period is observed. By integrating kinetic studies, heteronuclear Overhauser effect spectroscopy (HOESY) and density functional theory (DFT) calculations, we elucidate the key catalyst-solvent interactions governing the rates and aldehyde selectivity.

Track 2
Career Development

Chair: Jason Wu

Important Data for Your Project Sponsor Relationship

Annette A. Johnston, *AAJ Project Consulting LLC*

You will be working on projects, either as a graduate student, or working after graduation. It would seem straightforward to set up your project based upon a published charter, or direction from someone assigning the project to you. The standard process and guides will be reviewed during the presentation. Following this process will not be enough when issues out of your control start to badly impact your project. Remember that all projects have some adversity, and one of the key ways to work through adversity is to have complete support of the sponsor. The sponsor is the person or entity that provides the budget and resources for your project. It is critical to understand, before the project begins, how important the project is to the sponsor. In order to make risk management and communication plans, learn if they are prepared to fund or influence what is needed when uncontrollable adversity happens. During this presentation, some facts to collect from the sponsor are given, as well as how to use the information to set up and manage communication for the project.

Compensation Trends and the Job Market for Chemical Engineers

Adam Krueger, *Sun Recruiting*

I've been producing a compensation report specifically for Chemical Engineers in the United States for about 10 years. This presentation will be about that report, this year's results, trends over the past few years and how that relates to the overall job market for chemical engineers in the United States.

Track 3
Circularity & Sustainability

Chair: Gengnan Li

Analysis of the Environmental Impacts and Plausible Recyclability Effects of Additives in Plastics

Ulises R. Gracida-Alvarez, Pahola Thathiana Benavides, Troy Hawkins, *Argonne National Laboratory*, Gonzalo Rodriguez-Garcia, Kneifel Joshua, Sindhu Ranganath, *National Institute of Standards and Technology*

Additives are extensively utilized to enhance the properties of plastics, improving their processability and enabling them to meet specific requirements for various applications. While additives are essential in most plastic formulations, their impact on the greenhouse gas (GHG) emission of plastics is often neglected. Moreover, some additives are regulated due to health hazards and toxicological effects, which may limit their use and hinder the recycling of products that contain them. Reducing the concentration of these additives to the minimum amount for their technological performance could improve the recyclability of plastic products. Therefore, to explore these issues this study conducted a life cycle assessment to evaluate the environmental impacts of eight selected additives, including plasticizers, flame retardants, stabilizers, and pigments. The influence of these additives was assessed by incorporating them into the formulation of five different PVC products. The results indicate that the inclusion of specific additives in the selected PVC products may lead to an increase in GHG emissions between 0.3% to 25% compared to PVC without additives. The mass fraction of the additives showed a more significant impact than their inherent GHG emissions. Regarding recyclability, the study performed a hypothetical analysis to assess potential improvements in the closed-loop recycling of PET bottles. The outcome of this analysis suggested a possible increase in the recycling content of PET bottles by up to 12%, which could result in up to an 8% reduction in the use of virgin PET, based on the assumed increment in closed-loop recycling.

Plasma-Assisted Low Temperature Low Pressure CO2 Conversion to E-Fuels

Ghassan Alshehry, Hassan Alqahtani, Khalid Ruwaili *Saudi Aramco*

Synthetic fuels and chemicals are an inevitable building block towards achieving a net zero future. However, the cost and energy requirement of their production, attributed to the high stability of CO_2, hinders their adoption on a wider scale without the strict regulations put by governments. The scope of this paper it to propose plasma-assisted reactions, a cheap and energy efficient alternative, for CO_2 hydrogenation and syngas production.

Non-thermal plasma introduces viable reaction route to address carbon utilization and conversion into high value products, such as E-methanol and E-methane. E-methanol arises as a valuable option to convert and utilize captured carbon dioxide. It has the advantage of being the simplest alcohol and is in high demand as a fuel, a chemical, and an intermediate. Typically, the CO_2 hydrogenation to E-methanol requires extreme conditions sometimes exceeding 4 MPa and 200 ^oC. The presence of plasma can create a fertile environment for such reactions, due to the generation of excited electrons, charged ions and radicals. Wang et al. were able to produce a methanol yield of 11.3% at room temperature and atmospheric pressure, which marks a milestone in carbon capture and utilization (CCU) applications. In this review paper, we will address more potential NTP applications in carbon utilization, as well as a comparison of their energy requirement and cost when compared with conventional thermal reactions.

The goal is to accelerate the production of synthesis gas and low-carbon products including ammonia, methanol, and others. Plasma-assisted CO_2 conversion have shown high potential for CCU applications.

Afternoon Keynote

Global Race for A Better Battery

Prof. Y. Shirley Meng, UChicago, Argonne National Lab

Energy Storage Research Alliance (ESRA), Argonne National Laboratory, IL, USA
Laboratory for Energy Storage & Conversion, The University of Chicago, IL, USA

High energy long life rechargeable battery is considered as the key enabling technology for deep de-carbonization. Energy storage in the electrochemical form is attractive because of its high efficiency and fast response time. Besides the technological importance, electrochemical devices also provide a unique platform for fundamental and applied materials science & research since ***ion*** movement is often accompanied by inherent complex phenomena related to phase changes, electronic structure changes and defect generation. Synchrotron x-ray characterization plays critical role in understanding the ion transport, the dynamic structural changes and the corresponding degradations in high energy rechargeable batteries.

In this talk, I will discuss a few new perspectives for energy storage materials including new superionic conductors, new intercalation compounds and their interfacial engineering. With recent advances in photon and electron characterization tools and computational methods, we are able to explore ionic mobility, charge transfer and phase transformations in electrode and electrolyte materials *in operando* in materials beyond simple intercalation. Most recently we established ESRA, Energy Innovation Hub funded by the U.S. Department of Energy (DOE) focused on energy storage beyond lithium ion. ESRA aims to enable transformative discoveries in materials chemistry, gain a fundamental understanding of electrochemical phenomena at the atomic scale, lay the scientific foundations for breakthroughs in energy storage technologies, and train the next-generation battery workforce to ensure U.S. scientific and economic leadership.

Session 3

Track 1
Catalysis II

Chair: Trevor Lardinois
Co-Chair: Soroush Almassi

Exploring the Influence of Low Pt Loadings on Overlayered Mo-Nitrides for Selective Hydrogenation

Siobhan Brown, Justin Notestein,
Northwestern University

Overlayered, or, 'inverse' catalysts have seen increased interest for their attractive properties such as increased reducibility, increased reaction rates, selectivites, and altered electronic properties. The potential for an overlayered transition metal nitride catalyst was explored by the model system of MoNx/Pt/Al2O3. This nitrided material proved to exhibit similarly increased reducibility as seen in overlayered-oxides but, was not found to form the nitride at lower temperatures than the undoped material. Synergistic interaction(s) between the MoNx and Pt were found to be exist even when physically separated on the catalyst surface after high temperature ammonolysis. The potential as a hydrogenation catalyst was explored with CO chemisorption and ethylene hydrogenation as a probe reaction. Various pre-treatment of the catalyst resulted in two differing time on stream behaviors, deactivation and rates. The results of the MoPt material and further context will be discussed in this presentation.

Competitive Valerate Binding Enables RuO_2-Mediated Butene Electrosynthesis in Water

Špela Kunstelj, Andrea Darù, *University of Chicago*

Green hydrogen demands the use of water as the ultimate proton source. This reductive process requires the development of compatible electrooxidative half-reactions to simultaneously produce value-added products. The (non)-Kolbe electrooxidation of biogenic carboxylic acids, such as valeric acid, provides a sustainable synthetic route to access commodity products, like butene. The role of the electrode surface

in mediating the electron transfer in the reaction mechanism, which involves the oxidative and decarboxylative cleavage of a C–C bond preceding product formation, remains an open question; oxidative cleavage can either occur via an inner-sphere or outer-sphere electron transfer. Here, we present the electrochemical, in-situ spectroscopic, computational, and reactivity studies of RuO_2-mediated oxidative decarboxylation of valeric acid in aqueous alkaline electrolyte. We spectroscopically observe valerate binding at potential values where decarboxylation products are detected. Moreover, our results show that the competitive and catalytic oxygen evolution reaction (OER) is impeded by these bound carboxylate species. Our results suggest that valerate decarboxylation proceeds through an outer-sphere electron transfer mechanism, where the surface chemistry of the RuO_2 electrode suppresses the parasitic OER, which serves to enable higher non-Kolbe reaction selectivity. These findings outline design principles for selective electrosynthetic systems for sustainable oxidative decarboxylation compatible with water as the solvent. Our results highlight the synergy between in-situ experiments and computation to advance decarbonization chemistries.

In Situ Kinetic Analysis of Plasma-Enhanced Strong Metal-Support Interactions

Russell J. Clarke, Jason Hicks, *University of Notre Dame*

Inducing strong metal-support interactions (SMSI) is a well-established means to improve both the selectivity and stability of heterogeneous catalysts for industrially relevant reactions such as dehydrogenation. However, relatively extreme thermal conditions (~500°C) are required to induce the SMSI state, limiting its industrial potential and driving research efforts toward the discovery of alternative induction methods. Our recently published work successfully achieved the SMSI state and formed a Pt-Nb alloy in Pt/Nb_2O_5 using nonthermal plasma activation (termed P-SMSI) at temperatures as low as -30°C. Using a custom in situ FTIR cell with cryogenic plasma capabilities, we were able to collect time-resolved information on the formation of the NbO_X overlayer associated with P-SMSI, yielding a plausible mechanism and an associated rate law. The findings suggest that P-SMSI formation is diffusion controlled at low temperatures owing to the strong temperature dependence of surface diffusion compared to the weak temperature dependence of plasma-driven steps. Finally, the P-SMSI catalysts demonstrated enhanced selectivity to propylene in nonoxidative propane dehydrogenation compared to the untreated catalyst, highlighting the potential of P-SMSI as a catalyst promoter for commercial use.

Track 2
Bio Engineering

Chair: Meltem Urgun Demirtas
Co-Chair: Pahola Thathiana Benavides

Recovery of Organic Acids from Processed Biomass Using Advanced Ionomers and Electrochemical Separations

Christopher Arge, *Pennsylvania State University*, Yupo Lin, *Argonne National Laboratory*, Revati Kumar, *Louisiana State University*, Matthew Jordan, *EnergyX*

Purifying organic acids from processed biomass is energy intensive. Electrochemical separations, such as electrodialysis (ED) and electrodeionization (EDI), are an enticing platform to collect valuable organic acids without the use of chemicals while also using less energy. Here, we show that imidazolium-type of anion exchange membranes and ionomer binders in ED and EDI promote organic acid anion transport while concurrently boosting selectivity over competing inorganic ions. To uncover the governing molecular interactions that account for the improved transport and selectivity, we deployed 2D NMR (e.g., NOESY) and molecular dynamics simulations. These tools reveal that organic acid anions are closer to the imidazolium cation groups in anion exchange ionomers when compared to the conventional quaternary ammonium cations used in commercial anion exchange ionomers. The organic acid anions in closer proximity to the ionomer favor faster shuttling across the ionomer backbone. This talk will close with our recent work to fabricate mixed matrix anion exchange membranes for selective phosphate removal from wastewater (i.e., to prevent eutrophication of water bodies from agricultural runoff).

Life-Cycle Analysis of Microalgae-Based Polyurethane Foams

Ulises R. Gracida-Alvarez, Pahola Thathiana Benavides, Jingyi Zhang, Troy Hawkins, *Argonne National Laboratory*, Matthew Wiatrowski, Ryan Davis, *National Renewable Energy Laboratory*

Polyols and isocyanates are the primary precursors of polyurethane (PU), which rely on fossil-based sources for their production. Expanding these sources by incorporating biobased feedstocks, such as triglycerides (TAGs) derived from microalgae, could enhance the domestic supply of these materials while reducing the environmental impacts associated with their production. Furthermore, due to the health risks associated with isocyanates, alternative production pathways have been developed at laboratory scale that avoid their use and mitigate these hazards. Despite these potential advantages of microalgae-based PU, there is still limited information on its environmental impacts. Therefore, this study conducts a life cycle assessment (LCA) to evaluate the environmental impacts associated with two production pathways for microalgae-based PU: (1) a pathway where TAGs are converted into polyols and subsequently to PU using isocyanates (Bio-PU), and (2) a pathway where TAGs are converted into PU without using isocyanates (Bio-NIPU). Both Bio-PU and Bio-NIPU are co-produced in a biorefinery that also generates biofuels. The study evaluated both product- and a biorefinery-level LCAs. The product-level LCA results indicate that the greenhouse gas (GHG) emissions of Bio-PU and Bio-NIPU are up to 79% and 58% lower, respectively, compared to their conventional counterparts. At the biorefinery level, the LCA shows that a biorefinery producing bio-PU and biofuels can achieve up to 35% reduction in GHG emissions compared to conventional products. Similarly, a biorefinery producing Bio-NIPU can reduce GHG emissions by up to 28% compared to conventional products.

Mitigating Bioaerosol Risks from Industrial Cooling and Wastewater Systems

William Celenza, Audrey Keightley, *Burns & McDonnell*

The majority of water use at oil refining and petrochemical facilities is for heat transfer as cooling water or steam, or directly in the process. Less than 10% of supplied water sees direct process use, with cooling tower makeup which is the sum of the evaporation, blowdown, and drift rates accounting for up to 90%. Cooling tower blowdown can also contribute over 75% of the total process wastewater, or dry weather flow.

In 1976, public health awareness underwent a significant shift when a new strain of bacteria infected hundreds of attendees at an American Legion convention in Philadelphia. A type of pneumonia (lung infection) now called Legionnaires' disease and a less serious illness Pontiac fever were discovered to be caused by a bacteria, now known as Legionella pneumophila, that was dispersed through aerosolized droplets from a cooling tower plume. Likewise, the contamination of blowdown and wastewater with pathogens is a concern for wastewater treatment plant operators, most recently with the COVID-19 pandemic.

While cooling towers and wastewater aeration systems are essential to the operation of industrial facilities, they can also foster the growth and dissemination of pathogen-containing microorganisms. Even more concern has risen with the increased use of reclaimed water for cooling and utility water operations. Industry is now concerned with identifying and controlling the origins of bioaerosols. In the absence of regulations for managing bioaerosol risks, this presentation will review methods and practices currently used to lessen health risks from operation of cooling and wastewater systems at industrial facilities.

Track 3
Circularity & Sustainability II

Chair: Gengnan Li

Dynamic Simulation of CO_2 Adsorption in Amine-Based Sorbents for Direct Air Capture

Dana Marinic, Janvit Terzan, Blaž Likozar, *National Institute of Chemistry, Slovenia*

Environmental concerns have driven the development of direct air capture (DAC) technologies to mitigate rising CO_2 levels. However, DAC remains one of the most expensive carbon capture methods due to its high energy consumption. To accelerate research and improve process efficiency, modeling has emerged as a promising tool for understanding and optimizing DAC systems. In particular, multiscale modeling allows for a comprehensive analysis of the process, ranging from molecular interactions at the nanoscale to unit design at the macroscale.

Various dynamic models have been used to study CO_2 behavior in fluids, on sorbent surfaces, and within porous structures. Adsorption is described through equilibrium and dynamic aspects, including kinetics, mass, and heat transfer. Equilibrium is typically modeled using isotherms, while kinetics are captured by reaction rate equations or linear driving force (LDF) models. However, each model has strengths and limitations. Some isotherms overlook system heterogeneity, while others are empirical and modified to better fit experimental data rather than being derived from first principles. Likewise, kinetic models describe reaction rates but ignore mass transfer effects. This study compares multiple models to assess their predictive accuracy for CO_2 adsorption on amine-based sorbents.

A Techno-Economic Analysis of Virgin Lithium Compounds Production from Conventional Pathways

Sabine Gallagher, Qiang Dai, Nighat Afroz Chowdhury, Jeffrey Spangenberger, *Argonne National Laboratory*

The critical material lithium plays a vital role in fleet electrification and energy storage solutions. With this techno-economic analysis of lithium carbonate (Li_2CO_3) and lithium hydroxide monohydrate ($LiOH{\cdot}H_2O$) production we explored the total cost of production with comprehensive insights into differences in manufacturing routes and lithium resources. The study examines in detail current practices of mining and extraction operation as well as unit level operation in the refining process, and develops bottom-up cost models for the production technologies. Our analysis shows that in the traditional ore and brine route of Li2CO3 production, a total cost of \$10.48 and \$5.59 kg^{-1}, respectively is anticipated, including the cost of transportation between the mining or extraction site and the refining location. In comparison, The total cost of LiOH.H2O is estimated to be \$10.28 and \$6.13 kg^{-1}, for production from ore and brine respectively. Our analysis also estimates a carbon footprint of 14.1 kg CO_2e kg^{-1} for Li_2CO_3 from ore and 5.4 kg CO_2e kg^{-1} from brine, 14.4 kg CO_2e kg^{-1} for $LiOH{\cdot}H_2O$ from ore and 8.9 kg CO_2e kg^{-1} from brine. Moreover, this study includes sensitivity analysis of production locations including Australia, China, Chile and U.S. Furthermore, the ore grade as well as the brine concentration has been explored with a suggested cut off grade for each for the production routes to remain economically viable. The results of this study will pave the way to explore more innovative, domestic manufacturing processes in future for their environmental impact and cost competitiveness.

Poly(3-hydroxybutyrate)-Laminated Trilayer Composite Film for Active Food Packaging Application

Shu Xu, Kuang-Hao Cheng, Andrew Erwin, Wei Chen, Chaoyi Ba, Meltem Urgun-Demirtas, *Argonne National Laboratory*

Current environmental issues, such as plastic pollution and the high quantities of food waste, highlight a potential opportunity for utilizing food waste-derived feedstocks, specifically polysaccharides, in the production of disposable food packaging. Polysaccharides, however, possess an intrinsic hydrophilicity that creates considerable obstacles, such as diminished water vapor transmission and mechanical strength, when compared with petroleum-based plastics. In this work, dynamic covalent bonds were employed to achieve reversible crosslinking within

chitosan/starch blend films. Acetoacetate functional groups were used to modify starch, enabling a reversible reaction with the primary amine groups of chitosan. The excellent mechanical properties of chitosan were maintained in these films by using reduced starch concentrations relative to chitosan. Laminating a plasticized Poly(3-hydroxybutyrate) layer substantially decreased the water vapor transmission rate of the chitosan/modified starch layer. Further reduction of up to 99% compared to the single-layer chitosan/modified starch film was observed in trilayer films with two Poly(3-hydroxybutyrate) lamination layers. Incorporating β-carotene into the middle layer served as both an active ingredient and a photoprotective element. With no delamination observed during tensile testing, this multilayer lamination approach proved to be a successful method for enhancing the characteristics of polysaccharide films.

Session 4

Track 1
Catalysis III

Chair: Trevor Lardinois
Co-Chair: Soroush Almassi

Tandem CO_2-Oxidative Propane Dehydrogenation By in_2O_3-Overcoated Pt Catalyst

Geunho Han, Selim Alayoglu, Kunmo Koo, Justin Notestein, *Northwestern University*

Propane oxidative dehydrogenation can increase equilibrium conversion of highly endothermic propane dehydrogenation by consuming product, hydrogen, with oxidants, pulling the equilibrium to have a higher yield of propylene. Oxidants can be strong O_2 molecules as well as soft CO_2 molecules, which determines the subsequent oxidation reactions such as selective hydrogen combustion or reverse water gas shift. We designed catalysts to have multiple active sites (herein Pt and In_2O_3) on a single catalyst to perform multiple reactions simultaneously. Atomic layer deposition (ALD) was applied to powder chemistry to control nanometer-scale conformal deposition of metal oxides. We deposited a few layers of In_2O_3 onto Al_2O_3 supported Pt catalyst to build an "overcoated" structure. The overcoated nanocatalysts offer not only multiple reactive species but also unique properties, herein their interfaces. The addition of In_2O_3 significantly improved both CO_2 reduction and hydroformylation reactivity subsequent to propane dehydrogenation, and the overcoated structure strengthened the effect. Four different models of Pt and In_2O_3 were designed to unveil how two active sites facilitated the following reaction. A closer proximity between the active sites facilitated the kinetics of the tandem reaction. The findings demonstrated the evidence of kinetic coupling within the tandem system, unlike two individual kinetics working separately. To take advantages, individual catalytic components can be modified based on the purpose of catalytic reactions by exploiting kinetics.

Molybdenum Nitride on Platinum-Alumina for Ammonia Synthesis

Vinita Dubey, *Northwestern University*

Ammonia synthesis is critical for agriculture and industry, but it is energy intensive due to the high activation energy required for nitrogen reduction over existing catalysts. Metal nitrides have been proposed as alternatives to conventional Fe- or Ru-based catalysts, but these often have low rates of ammonia release. This study explores strategies for promoting a MoN_x supported on Al_2O_3. The primary objectives were to determine the structure of the synthesized material, evaluate nitrogen uptake capacity, examine the accessibility of lattice nitrogen, and investigate the role of Pt in promoting catalytic activity through hydrogen dissociation and spillover effects. XRD confirmed the formation of a Mo_2N phase and temperature programmed reduction (TPR) revealed that Pt incorporation significantly enhances the reducibility of the starting Mo oxide and increases the amount of removable N from the nitride from 6.7% to 19.3% which indicates the availability of N_2 vacancy. MoN_x/Pt catalyst shows improved ammonia rates at low temperatures. The enhanced performance was attributed to enhancement of a Mars-van Krevelen mechanism, where lattice nitrogen participates directly in the reaction cycle, facilitated by Pt's ability to dissociate hydrogen and reduce the energy barrier for nitrogen

activation. These results provide new insights into the design of nitride-based catalysts, demonstrating that the synergy between Pt and MoN_x can significantly improve ammonia synthesis under mild conditions. This work is expected to be of interest to researchers aiming to develop energy-efficient catalytic systems for ammonia synthesis considering the reducibility aspect of the nitride-based catalyst.

Ethylene and Propylene Co-Oligomerization in Mesoporous Catalysts

Alba Scotto d'Apollonia, Jason Hicks,
University of Notre Dame

Light olefin oligomerization is a key reaction in the modern economy, as oligomers are used for the production of chemicals and commodity products. The C–C coupling of olefins can be catalyzed by transition metals, with nickel being the most commonly used active site. Its primary application is in homogeneous oligomerization, owing to its high activity in ethylene conversion and selectivity to linear products. While the fundamental aspects of oligomerization have been extensively studied, reactions involving mixed feeds remain underexplored, despite the widespread occurrence of olefin mixtures in various applications. Understanding the kinetics of mixed olefins can help elucidate the accessible pathways within the catalyst pores, thereby facilitating the design of more efficient catalysts and processes. In this work we investigate the oligomerization of ethylene-propylene mixtures over Ni^{2+} active sites dispersed on mesoporous silica, using tungsten-oxide polyoxometalates as platforms to prevent nickel migration. Our findings uncover conditions where ethylene oligomerization turnover rates can be promoted due to potential stabilization effects. Additionally, with the goal of integrating our observations on mesoporous catalysts with microporous materials, this study extends also to nickel over zeolite catalysts (e.g. BEA). Further, we explore the product distributions at different operating conditions and pore size, providing insights on the mechanism of co-oligomerization with mixed feeds.

Track 2
Process Systems/AI/ML

Chair: David Neira
Co-Chair: Shri Dawande

Process Modeling and Techno-Economic Optimization for Production of Lignin-Isolated Soy Protein-Based Bio-Adhesive

Poulomi Das, Debangsu Bhattacharyya, Changle Jiang, Jianli Hu, *West Virginia University*

To date, many chemicals, including adhesives, have been produced from fossil sources, leading to environmental concerns; thus, spurring interest in replacing them with bio-derived alternatives that offer reduced environmental footprints and enhanced sustainability. Currently, global wood panel industry primarily relies on petroleum-based adhesives like phenol-formaldehyde, urea-formaldehyde, etc. They emit toxic volatile organic compounds, e.g., formaldehyde, which can cause severe health issues.

Soy-protein adhesives offer a biodegradable, low-cost, and high-production formaldehyde-free alternative to these synthetic adhesives. However, they suffer from low water resistance and weak bonding strength. Furthermore, lignin can be considered another potential raw material for bio-adhesive due to the presence of both alcohol- and phenol-type hydroxyl groups in its complex molecular structure. Crosslinking lignin with soy protein improves adhesive performance. In the proposed technology, the manufacturing process is divided into two steps – (1) partial depolymerization of KL; (2) addition of the KL oligomer fragments to SPI to produce lignin-isolated soy protein bio-adhesive.

This work discusses the development of a detailed kinetic model for the thermochemical degradation of KL through the base-catalyzed depolymerization (BCD) method, and the simultaneous estimation of optimal kinetic parameters using in-house experimental information. Subsequently, we propose a plant-wide model for the production of lignin-soy protein isolate-based bio-adhesive. The lab-scale reactor model has also been scaled up to the commercial scale. An economic model of the whole process has been

developed involving mathematical optimization of the design parameters and operating conditions for the reactors with the objective of maximizing the net present value (NPV).

Computational Optimization and Machine Learning Modeling of Membrane-Assisted Bio-Methanol Dehydration

Hamta Bardool, *Purdue University*, Andres Cabeza, *Universidad Nacional de Colombia*, Sede Bogotá, David E. Bernal Neira, *Universities Space Research Association*

The membrane-assisted dehydration of bio-alcohols is an effective method for producing sustainable biofuels and chemical intermediates. (Bakhtyari et al., 2023) This study develops a detailed mathematical model for bio-methanol dehydration, incorporating reaction kinetics, transport phenomena, and thermodynamic constraints. The membrane system improves conversion by selectively removing water during the reaction, shifting the equilibrium toward higher dimethyl ether (DME) yields and reducing separation costs.
To enhance process efficiency, a cost-focused optimization framework is applied using Pyomo DAE, (Nicholson et al., 2018) aiming to reduce operating expenses while maintaining high conversion and selectivity. Key parameters, such as pressure, temperature, and sweep gas flow rate, are optimized to identify the most cost-effective conditions. In addition, machine learning techniques are used to develop predictive models based on Physics-Informed Neural Networks (PINNs) (Karniadakis et al., 2021) and Karush-Kuhn-Tucker-enhanced PINNs (KKT-hPINNs). (Chen et al., 2024) These models are trained on a dataset generated from Aspen Custom Modeler (ACM) simulations, allowing accurate predictions of reactor performance. Results show that KKT-hPINNs perform better than conventional neural networks, providing higher accuracy, lower error rates, and strict adherence to physical laws.
By combining Pyomo DAE-based optimization with machine learning-based modeling, this study presents an efficient computational approach for improving reactor performance. The results highlight how advanced optimization and artificial intelligence can reduce costs, enhance efficiency, and support the transition to sustainable biofuel production.

Introducing a Bayesian Approach for Sparse Modeling of Time-Delayed Process Systems

Samuel Adeyemo, *Calvin University*, Debangsu Bhattacharyya, *West Virginia University*

Data-driven model building for time delay systems is difficult due to noise in the data, unknown delays in each input and output variables used for model building, and nonlinear dynamics. This is particularly challenging for developing sparse, interpretable data-driven models using well-defined basis functions when the training data contain noise with unknown characteristics.
In this work, we develop a systematic approach for building sparse, interpretable, dynamic models. The approach develops a novel Bayesian Identification of Dynamic Sparse Algebraic Model (BIDSAM) algorithm that can optimally select the optimal basis functions from a set of candidate basis function, optimally estimate the model parameters through Bayesian inference, and optimally estimate time delays in inputs/outputs. An efficient bidirectional branch & bound algorithm is developed to solve the MINLP problem. By testing on two case studies, we show that the proposed approach gives sparse models estimating the unknown time delays with 80% accuracy while keeping prediction RMSE below 5%.

Development of an Online Health Monitoring Framework for High-Temperature Boiler Components by Using Hybrid First Principles-Artificial Intelligence Models

Vivek Saini, *West Virginia University*, Angan Mukherjee, *University of Wisconsin-Madison*, Samuel Adeyemo, *Calvin University*, Debangsu Bhattacharyya, *West Virginia University*

The increasing integration of renewables into the energy grid requires fossil-fired power plants to operate flexibly, leading to frequent load changes that stress critical boiler components. These dynamic operations accelerate component damage, affecting reliability and increasing operational costs. To maintain efficiency, adaptive condition monitoring tools that generalize across plant configurations are essential for recognizing

load-following impacts, improving safety, and preventing outages.

This work presents a health monitoring framework for high-temperature boiler components, combining first principles (FP) physics-based and artificial intelligence (AI) models. While FP models offer accurate predictions, they are computationally expensive, whereas AI models are faster but often lack accuracy in nonlinear systems. High-temperature boiler components, like steam superheaters, have complex dynamics with limited measurements of critical variables, such as metal wall temperatures, which can be useful for estimating metallurgical changes like oxide scale formation. Since direct measurement of oxide scale thickness inside tubes is impractical, hybrid models can be useful for predicting the spatio-temporal profile in these components.

This work developed two hybrid model structures: one integrating AI with FP models in series for specific phenomena and another using a parallel approach to capture spatial temperature variations. The FP model employs a dynamic, distributed 3D differential-algebraic equation (DAE) framework, while the AI model uses static-dynamic neural networks and Bayesian techniques. The framework was validated using oxide scale measurements from a coal boiler superheater using 23 months of operational data, demonstrating its effectiveness in predicting boiler component health under load-following operations, optimizing maintenance, and improving power plant reliability.

Track 3
Energy Storage

Chair: Mohammed Effat

Cost Modeling of Cathode Active Materials in Electric Vehicle Batteries

Kevin Knehr, Joseph Kubal, Shabbir Ahmed, *Argonne National Laboratory*, Licheng Su, Nicholas Neu, Kyle Gordon, *Roland Berger*

The growing adoption of electric vehicles has created a dynamic market that is impacted by new chemistries, new technologies, and supply chain uncertainty. Technoeconomic models are essential tools for forecasting how these new trends and uncertainties will impact the cost of battery packs. This study leverages a suite of models at Roland Berger and Argonne National Laboratory to assess the influence of new chemistries and changing raw material prices on the future cost of battery packs. PCAM and CAM production models are used to translate the price of raw materials into active material costs when manufactured at scale within the United States. The Battery Performance and Cost (BatPaC) Model at Argonne National Laboratory is used to translate these CAM prices into battery pack cost for a range of electric vehicles. The study highlights the main factors controlling pack costs and provides insight into future trends.

Powering the Future: Challenges and Opportunities in Electrical Generation

Maria Salazar, *Chemistry in Business and Education*

This presentation will describe the technological challenges that countries around the world are facing to meet the energetic demands of their populations with out impacting the environment. While most countries rely on fossil fuels, others are using alternatives sources of energy, for example geothermal or nuclear. The importance of using renewable fuels will be emphasized. New concepts that push the boundaries of science and technology will be presented, from space solar power generation to microbial fuel cells.

Impact of Thermal Gradients on the Dynamics of Cylindrical Lithium-Ion Cells and the Module

Mohammed Effat, Joseph Kubal, Kevin Knehr, Shabbir Ahmed, *Argonne National Laboratory*

A comprehensive model has been developed to evaluate how different thermal gradient patterns, created by various cooling plate (CP) designs, impact the dynamics of a module containing cylindrical lithium-ion cells. This model integrates computational fluid dynamics (CFD), a pseudo-two-dimensional (P2D) battery model, cell aging due to solid-electrolyte-interphase growth, and electric current distribution from module terminals to cells. Three CP designs—straight, perpendicular, and U-turn—were analyzed

alongside three electrical configurations: parallel-connected strings, series-connected cells, and a combination of both. The study examined how thermal gradients affect resistance, current, state of charge, and voltage variability among cells. Results showed that in parallel-connected strings, the self-balancing nature counteracted resistance variation effects coming from thermal gradients, unlike in series-connected cells, where voltage imbalances from thermal gradients led to performance deterioration. The worst performance was observed in modules with thermal gradient applied to both series and parallel connected cells, especially at large thermal gradients (e.g., Δ10 °C). The study highlights the importance of considering the pattern of thermal gradient in selecting a CP for lithium-ion battery modules.

Evening Keynote

Perspectives of Quantum Computing in Chemical Engineering

Prof. David Neira, Purdue University

As part of the UN International Year of Quantum, we are happy to share some perspectives of the use of quantum computing for chemical engineering. Quantum technologies have attracted a considerable interest of the federal, state, and city governments in the US, Illinois, and Chicago respectively, leading to Chicago becoming one of the major hubs in the advancements in quantum science and technology. Quantum computing has also been attracting public attention recently. This interest is driven by the advancements in hardware, software, and algorithms required for its successful usage and the promise that it entails the potential acceleration of computational tasks compared to classical computing. This perspective talk presents a review of quantum computing, how this computational approach solves problems, and three fields that quantum computing can potentially impact the most while relevant to chemical engineering: computational chemistry, optimization, and machine learning. Here, we present a series of chemical engineering applications, the developments, potential improvements concerning classical computing, and challenges that quantum computing faces in each field. The first part of this talk intends to provide a clear picture of the challenges and potential advantages that quantum technology may yield for chemical engineering, together with an invitation for our colleagues to join us in the adoption and development of quantum computing. This part corresponds to the recent invited publication on Perspectives on Quantum Computing for Chemical Engineering at the AIChE Journal https://doi.org/10.1002/aic.17651 and received the best talk award at the Quantum Computing Applications in Chemical and Biochemical Engineering Workshop at Copenhagen.

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- Energy Storage I
Chair: **Mohammed Effat (Argonne National Laboratory)**

- Poster Session
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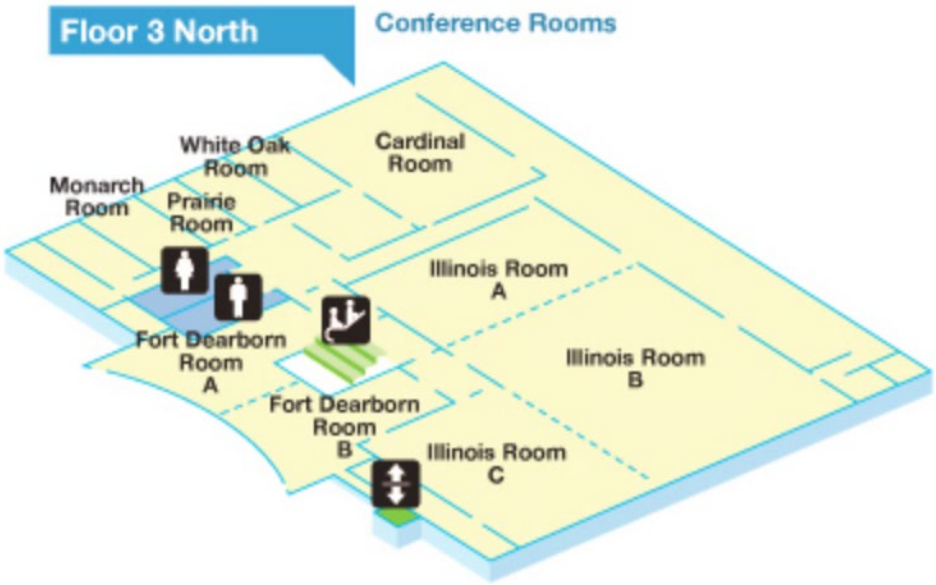
Conference Map

Directions to UIC Student Center East:

1) The conference will be held on **Floor 3 North** of the **UIC Student Center East** (750 S Halsted St, Chicago, IL 60607).

2) Paid parking is available across the street in the **Halsted/Taylor Parking Structure** (760 W Taylor St, Chicago, IL 60607). Entrance is from Taylor Street.



Room	Description
Cardinal Room	Morning and Afternoon Keynote Track 3
White Oak Room	Track 1
Illinois Room C	Track 2
Illinois Room B	Conference Introduction Lunch + Dinner Evening Keynote
Illinois Room A	Poster Session
Fort Dearborn Room AB	Breakfast/Registration/Coffee Breaks Sponsor Exhibits

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