DRAFT PROGRAM- 3/31/2023

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MIDWEST REGIONAL
CONFERENCE

15th Annual
AIChE Midwest Regional Conference

April 11-12, 2023
University of Illinois at Chicago
(Student Center East)
https://www.aiche.org/conferences/midwest-regional-conference/2023

Organized by the AIChE Chicago Local Section
Hosted by the University of Illinois at Chicago

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Conference Overview

The AIChE Midwest Regional Conference (MRC) continues into its 15th year. Organized by the **AIChE Chicago Local Section, AIChE Global** and the **University of Illinois 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:

4 Keynote Lectures:

- **Rep. Sean Casten,** *U.S. Congressman for the 6th District of Illinois*
- **Susan Babinec,** *Program Lead – Stationary Storage, Argonne National Laboratory*
- **Dr. Quinta Warren,** *Associate Director of Sustainability Policy, Consumer Reports*
- **Dr. Frank Zhu,** *Senior Fellow, Honeywell UOP*

The conference contains **14 technical sessions** featuring **46 oral presentations and multiple posters.** The Tuesday evening program is combined with the ***AIChE Chicago Local Section Monthly Meeting*** for dinner, keynote, and meeting.

The conference also features a **Student Outreach Program**, where Chicago-area high school students will become acquainted with the various facets of the chemical engineering profession. The High School Outreach program features **Valarie King-Bailey, MBA** (CEO of OnShore Technology Group) as keynote speaker and includes an in-person lunch where students can interact with practicing engineers.

On behalf of the conference planning committee, we welcome you to the 15th Annual AIChE Midwest Regional Conference and hope you will take advantage of all the opportunities it has to offer.

Jessica Morris
Conference Chair
Senior Associate, Exponent

Belma Demirel
Conference Co-Chair
Process Engineer, bp

Hakim Iddir
Technical Program Chair
Physicist, Argonne National Laboratory

Jason Wu
Technical Program Co-Chair
Lead R&D Engr/Scientist Honeywell UOP

Program at a Glance (Day 1)

Tuesday, April 11th, 2023

8:45 – 9:00 AM	**Conference Introduction**	
9:00 – 10:00 AM	**1st Morning Keynote** (Cardinal Room) Rep. Sean Casten, *U.S. Congressman for the 6th District of Illinois*	
10:00 – 10:15 AM	**Networking Break**	
10:15 – 11:15 AM	**2nd Morning Keynote** (Cardinal Room) Susan Babinec, *Argonne National Laboratory*	
11:15 AM – 12:15 PM	**Lunch** (Illinois AB)	
	Track 1 (White Oak Room)	**Track 2** (Illinois C)
Session I	12:15 – 1:30 PM *Energy Storage I*	12:15-1:05 PM *Process Safety*
Networking Break (Dearborn A/B)	1:30 – 1:45 PM	1:05- 1:20 PM
Session II	1:45 – 3:00 PM *Energy Storage II*	1:20 – 3:00 PM *Environmental Compliance / Remediation*
Networking Break (Dearborn A/B)	3:00 – 3:15 PM	3:00 – 3:15 PM
Session III	3:15 – 4:55 PM *Advances in Refining & Biorefining*	3:15 – 4:55 PM *Green Engineering*
4:55 – 5:45 PM	**Poster Session/Networking Break** (Illinois AB)	
5:45 – 7:30 PM	**Chicago Section Monthly Technical Dinner** (Cardinal Room) **Dinner Keynote** – Dr. Quinta Warren, *Consumer Reports*	

Program at a Glance (Day 2)

Wednesday, April 12th, 2023

8:45 – 9:00 AM	**Conference Introduction** (Cardinal Room)	
	Track 1 (White Oak Room)	**Track 2** (Illinois C)
9:00 – 10:15 AM	**Session I** *Bioengineering & Nanotechnologies*	*Machine Learning & Optimization*
10:15 – 10:30 AM	**Networking Break** (Dearborn AB)	
10:30 – 11:20 AM	**Session II** *Bioengineering and Nanotechnologies*	*Machine Learning & Optimization*
11:20 AM – 12:45 PM	**Networking/Lunch Break** (Cardinal Room)	
12:45 – 1:45 PM	**Afternoon Keynote** (Cardinal Room) Dr. Frank Zhu, *Honeywell UOP*	
1:45 – 2:00 PM	**Networking Break** (Dearborn AB)	
2:00 – 3:15 PM	**Session III** *Catalysis I*	*Fluid Properties, Fluid Dynamics & Transport Phenomena*
3:15 – 3:30 PM	**Networking Break** (Dearborn AB)	
3:30 – 4:45 PM	**Session IV** *Catalysis II*	*Polymers*
5:00 – 8:00 PM	**Happy Hour Hosted by Chicago Local Section (CLS) Young Professionals (YP)**	

Keynote Speakers

***Tuesday Morning Keynote*: 9:00 AM April 11, 2023**

Rep. Sean Casten, *U.S. Congressman for the 6th District of Illinois*

As a scientist, clean energy entrepreneur and CEO, and now as a Member of Congress, Representative Sean Casten has dedicated his life to fighting climate change. In Congress, Casten draws on his two decades of experience as a business leader to reduce emissions while creating jobs, lowering energy costs for Americans, and spurring economic growth. Casten serves on the House Financial Services Committee and the Science, Space, and Technology Committee. He also serves as Vice-Chair of the Sustainable Energy and Environment Coalition (SEEC). While working diligently in Washington on behalf of Illinois' 6th Congressional District, Rep. Casten is also committed to keeping in close contact with his constituents. He lives in Downers Grove with his family.

Visit Rep. Casten's website: https://casten.house.gov

***Tuesday Morning Keynote*: 10:15 AM April 11, 2023**

Susan Babinec, *Program Lead – Stationary Storage, Argonne National Lab*

Sue Babinec is the Program Lead – Stationary Storage at Argonne National Lab where she leads efforts ranging from new tools and capabilities to enhance existing technologies and breakthrough research for new approaches to long duration energy storage goals. Babinec previously served six years in Washington DC as senior commercialization advisor at the Advanced Research Projects Agency – Energy (ARPA-E) where she co-managed the energy storage portfolio for both transportation and grid. Prior to ARPA-E she led several research groups focused on design and scale-up of Li-ion technologies as a technical director for A123 Systems, Inc.. Babinec spent the first two decades of her career at The Dow Chemical Corp., where she was the Senior Electrochemist, a senior member of the Corporate VC group, was awarded the Inventor of the Year Award, and was the company's first woman Corporate Fellow. She holds 50+ patents and has authored or coauthored dozens of journal articles and book chapters.

Tuesday Dinner Keynote: 7:00 PM, April 11, 2023

Dr. Quinta Warren, *Associate Director of Sustainability Policy, Consumer Reports*

Dr. Quinta Warren is the Associate Director of Sustainability Policy at Consumer Reports (CR), where she leads the legislative, regulatory, and corporate engagement strategies for sustainability on behalf of consumers. She is the co-author of a major CR survey report on consumer attitudes toward electric vehicles and low carbon fuels. She recently testified before Congress about the consumer benefits of the historic clean energy provisions in the Inflation Reduction Act. She and her team have also worked closely with policymakers and consumers to advance reforms such as California's landmark Advanced Clean Cars rule and the federal government's new standards for fuel economy and emissions. Previously, Dr. Warren worked on carbon capture with ConocoPhillips, power generation with the Department of Energy, and international development with the Millennium Challenge Corporation and her own firm, Energy Research Consulting. Dr. Warren holds a PhD in Chemical & Biomolecular Engineering from Georgia Tech, and a Bachelors in Chemical Engineering from Penn State.

Wednesday Afternoon Keynote: 12:45 PM April 12, 2023

Dr. Frank Zhu, *Senior Fellow, Honeywell UOP*

Dr. Frank Zhu is a Honeywell-UOP Senior Fellow leading technology innovations and has made significant contributions to the fields of energy efficiency, operation optimization, and process modeling and design. Franks' methods have been successfully applied to industries and generated significant benefits in economic margin, energy savings and emission reductions. For example, he led design of several grassroots refineries and petrochemical complexes which are ranked in the category of the highest energy efficiency worldwide.

Frank was the recipient of the prestigious AIChE Energy Sustainability Award 2014 due to his contributions. Published several books and more than 100 papers and 60 patents granted.

Session Presentations (Day 1)

Tuesday, April 11, 2023

Conference Welcome

8:45 AM Conference Introduction (Cardinal Room)
Jessica Morris (Conference Chair, Exponent)
Belma Demirel (Conference Co-Chair, bp)

Tuesday Morning Keynote Sessions

9:00 AM **Keynote Introduction 1**
Jessica Morris (Conference Chair, Exponent)
9:05 AM _______NEED TITLE________________
Rep. Sean Casten (U.S. Congressman for the 6th District of Illinois)

10:15 AM **Keynote Introduction 2**
Jessica Morris (Conference Chair, Exponent)
10:20 AM **Energy Storage – How we got here, where are we going.**
Susan Babinec (Argonne National Laboratory)

Session I:

Track 1: Energy Storage I (White Oak Room)
Chair: *Juan Garcia* (Argonne National Laboratory)
Co-Chair: *Hakim Iddir* (Argonne National Laboratory)
12:15 PM **Study of Earth-Abundant, Mn-Rich Cathodes for Vehicle Applications and Beyond**
Jiajun Chen (Argonne National Laboratory)
12:40 PM **Na-Ion Delivery Via Molecular Cages in Porous Liquid Type-II Electrolytes**
Sakshi Singh (University of Illinois Chicago)
1:05 PM **Hybrid Air Conditioning Thermal Energy Storage for Space Cooling Applications**
Said Al-Hallaj (University of Illinois Chicago)

Track 2: Process Safety (Illinois C)
Chair: *Jessica Morris* (Exponent)
Co-Chair: *Nick Schulman* (Exponent)
12:15 PM **Process Safety in Hydrogen Industries**
William Giang (PSRG Inc.)
12:40 PM **PSM Pillars…or Dominos? A Case Study to Consider the Link between Certain PSM Pillars.**
Domingo Elias (Exponent)

Session II:

Track 1: Energy Storage II (White Oak Room)
Chair: *Hakim Iddir* (Argonne National Laboratory)
Co-Chair: *Juan Garcia* (Argonne National Laboratory)
1:45 PM **Structural Features in Li- and Mn- Rich Cathodes that Modify the Impedance at Low State of Charge**
Juan Garcia (Argonne National Laboratory)
2:10 PM **Role of Crystal Size in Dynamic Charge Acceptance of Lead-Acid Batteries**
Kevin Knehr (Argonne National Laboratory)
2:35 PM **Physics Informed Design of Porous Silicon Based Electrodes**
Abhas Deva (Argonne National Laboratory)

Track 2: Environmental Compliance / Remediation (Illinois C)
Chair: *Aditya Prajapati* (LLNL)
Co-Chair: *Taiwo Adesanya* (UIC)
1:20 PM **Removal of Fluoride from Water Using Hybrid Aluminum-Magnesium-Calcium Coated Sand Adsorbent**
Kiana Modaresahmadi (University of Illinois Chicago)
1:45 PM **Electrochemical Degradation of Perfluorooctanoic Acid Using Electrocatalytic Reactive Electrochemical Membranes**
Saurabh N. Misal (University of Illinois Chicago)
2:10 PM **Electrochemical Reduction Using Ti4O7 Reactive Membranes Impregnated with Nickel and Iron for Pfas Destruction** (TuB2c)
Jacob King (University of Illinois Chicago)
2:35 PM **A Mechanistic Study on per-and Polyfluorinated Substances (PFAS) Electrooxidation on Ti4O7 Anode**
Shirin Saffar Avval (University of Illinois Chicago)

Session III:

Track 1: Advances in Refining & Biorefining Technology (White Oak Room)

Chair: *Rishabh Jain* (Honeywell)
Co-Chair: *Belma Demirel* (bp)

3:15 PM **Life Cycle and Technoeconomic Analyses of Catalyst Used in the Conversion of Waste Plastic to Lubricate Oils from Upcycled Plastics (LOUPs)**
Pahola Thathiana Benavides (Argonne National Lab)

3:40 PM **Effective and Efficient Chemical Recycling of Waste Plastics Is Dependent on the Presence of Catalysts**
Jeff Martin (Ketjen)

4:05 PM **Status of Blue H2 and Blue Ammonia As the New Decarbonized Fuel of Today and the Future**
Jeron Chin (Haldor Topsoe)

4:30 PM **Gas Fermentation: New Process Technology for a Circular Carbon Economy**
Sean Rollag (LanzaTech)

Track 2: Green Engineering (Illinois C)

Chair: *Jason Wu* (Honeywell UOP)
Co-Chair: *Omar Aly* (UIC)

3:15 PM **Computational Screening of MOF and Working Fluid Pairs for Adsorption Cooling Applications**
Filip Formalik (Northwestern)

3:40 PM **Graph Neural Network Model to Predict Carbon Adsorption Capability of MOF**
Hyun Park (University of Illinois Chicago)

4:05 PM **Diffusion Model Accelerates Computational Design of MOF Structures for Carbon Capture**
Ruijie Zhu (Northwestern)

4:30 PM **Left or Right? Which Way on a Decarbonization Journey?**
Katelyn Tran (Wood Group USA)

Poster Session (Illinois B)

Chair: *Adam Kanyuh* (Honeywell UOP)
4:55 PM **Poster Session**

Chicago Section Monthly Technical Dinner and Dinner Keynote (Cardinal Room)

5:45 PM **Dinner**
6:15 PM **Section Announcements**
6:30 PM **Keynote Introduction**
(Belma Demirel, bp)
6:35 PM **The Consumer Case for Electric Vehicles**
Dr. Quinta Warren (Consumer Reports)
7:30 PM **Poster Presentation Awards**

Session Presentations (Day 2)

Wednesday, April 12, 2023

Conference Welcome

8:45 AM **Conference Introduction**
Jessica Morris (Conference Chair, Exponent)

Session I:

__Track 1: Bioengineering & Nanotechnologies__ __(White Oak Room)__
Chair: *Meltem Urgun-Demirtas* (Argonne National Lab)
9:00 AM **INSERT TITLE AND NAME**
9:25 AM **Will Future Generations of N95 Masks Include Atomic Layer Deposited Silver Nano-Islands?**
Harshdeep Bhatia (University of Illinois Chicago)
9:50 AM **Developing a Platform for Induced Pluripotent Stem Cell Reprogramming through Lipid Nanoparticle-Based mRNA Delivery**
Emily Kim (UPenn*)*

__Track 2: Machine Learning & Optimization__ __(Illinois C)__
Chair: *Aashutosh Mistry* (Argonne National Lab)
9:00 AM **Hybrid Series and Parallel All-Nonlinear Dynamic-Static Neural Networks: Development, Training, and Application to Chemical Processes**
Angan Mukherjee (WVU)
9:25 AM **Accelerating MOF Synthesis Via Data Mining and Machine Learning**
Manuel Tsotsals (Karlsruhe Institute of Technology)
9:50 AM **Small Molecule Adsorption Energy Predictions for High-Throughput Screening of Electrocatalysts**
Srishyam Raghavan (University of Illinois Chicago)

Session II:

__Track 1: Bioengineering& Nanotechnologies__ __(White Oak Room)__
Chair: *Meltem Urgun-Demirtas* (Argonne National Lab)
10:30 AM **Inter-Electronic and Inter-Valley Transitions in MoS2-WS2 Heterostructures and Alloys**
Sungjoon Kim (University of Illinois Chicago)
10:55 AM **Tunable Sulfur Incorporation into Atomic Layer Deposition Films Using Solution Anion Exchange**
Julia Lenef (University of Michigan)

__Track 2: Machine Learning & Optimization__ __(Illinois C)__
Chair: *Aashutosh Mistry* (Argonne National Lab)
10:30 AM **Generative Adversarial Network to Accelerate Computational Screening of Metal-Organic Framework Structures**
Xiaoli Yan (University of Illinois Chicago)
10:55 AM **Exploring MOF Sorption Properties with Topological Data Analysis**
Seth Moore (University of Chicago)

Afternoon Keynote Session (Cardinal Room)

12:45 PM **Keynote Introduction**
Hakim Iddir (Argonne National Laboratory)
12:50 PM **Integrating Multiscale Modeling and Optimization for Sustainable Process Development**
Frank Zhu (Honeywell UOP)

Session III:

__Track 1: Catalysis I__ __(White Oak Room)__
Chair: *Trevor Lardinois* (Exponent)
Co-Chair: *Nicole Libretto* (Honeywell)
2:00 PM **Amino Acid Glycine-Derived Metal-Free Nitrogen-Doped Ordered Mesoporous Carbon for Efficient Electrochemical Synthesis of Hydrogen Peroxide (H2O2)**
Basil Rawah (Illinois State University)
2:25 PM **Ligand-Coordination Effects on the Selective Hydrogenation of Acetylene in Single-Site Pd-Ligand Supported Catalysts**
Eman Wasim (Indiana University)
2:50 PM **First-Principles Analysis of the Ammonia Decomposition Reaction on High Entropy Alloy Catalysts**
Zuhal Cakir (Purdue University)

__Track 2: Fluid Properties, Fluid Dynamics, & Transport Phenomena__ __(Illinois C)__
Chair: *Hadjira Iddir* (Honeywell UOP)
2:00 PM **Performance of a CSTR Activated Sludge with Different Configurations for Municipal Wastewater Treatment**
Seyed Amirfakhri (University of Wisconsin)
2:25 PM **Obtaining Structural Information of Carbon Black in Carbon Black/Polyvinylidene Difluoride**

Suspensions with Simultaneous Rheo-Electric Measurements
Qingsong Liu (Northwestern)

2:50 PM **Modeling and Numerical Simulation of Concentrated Solar Energy Storage in a Packed Bed of Silicon Carbide Particles**
Zeyuan Gao (IIT*)*

Session IV:

Track 1: Catalysis II (White Oak Room)

Chair: *Nicole Libretto* (Honeywell)
Co-Chair: *Trevor Lardinois* (Exponent)

3:30 PM **Mechanistic Insight into Tris(pentafluorophenyl)Borane Speciation during Ring Opening of Epoxides**
Hiyab Mekonnen (Northwestern University)

3:55 PM **Non-Thermal Plasma Assisted Catalytic Water Splitting for Clean Hydrogen Production at Near Ambient Conditions**
Mingyuan Cao (Notre Dame)

4:20 PM **Deciphering Activity Controls for Ethylene Oligomerization Catalyzed By Metal Ions Grafted on Oxide Supports By Computational Interrogation**
Neha Mehra (Notre Dame)

Track 2: Polymers (Illinois C)

Chair: *Carina Martinez* (UIC)
Co-Chair: *Cheryl Slykas* (UIC)

3:30 **PM Molecular-Level Insights into the Diffusion Mechanism of a Hydrophobic Drug from a Block Copolymer Micelle By Molecular Dynamics Simulation**
Negin Razavilar (Kettering University)

3:55 PM **Upcycling Virgin and Waste Polyethylene to Reprocessable Dynamic Covalent Networks Via Free-Radical Grafting of Dialkylamino Disulfide Bonds**
Logan Fenimore (Northwestern)

4:20 PM **Rheology and Spinnability of Polyvinylpyrrolidone Solutions**
Louis Edano (University of Illinois Chicago)

Presentation Abstracts (Day 1)

Tuesday, April 11, 2023

Tuesday Morning Keynote Sessions

9:00 AM

TITLE OF TALK

Rep. Sean Casten (U.S. Congressman for the 6th District of Illinois)

INSERT ABSTRACT FOR TALK

10:15 AM

Energy Storage – how we got here, where are we going.

Susan Babinec (Argonne National Laboratory)

There has never been a better time to be involved in energy storage, which is now recognized as a key enabling technology in the urgent battle against climate change. Electrified transportation of light duty vehicles is the first new approach in 100 years and has been codified in many global policies – the next challenge is heavier vehicles, air and marine transport. Renewables are the dominant new power generation but require energy storage to manage their intermittency. Li-Ion has started this journey, but long duration energy storage is required to hit the deep decarbonization goals. The pace of change is high. We will review the interwoven science/market history of early developments and set the stage for what is to come in this presentation.

Session 1:
Track 1: Energy Storage I

Chair: Juan Garcia (Argonne National Lab)

Co-Chair: Hakim Iddir (Argonne National Lab)

12:15 PM

Study of Earth-Abundant, Mn-Rich Cathodes for Vehicle Applications and Beyond

Jiajun Chen (Argonne National Lab)

Lithium- and manganese-rich (LMR) oxides are attractive candidates as cathode materials for next generation lithium-ion batteries due to their high capacities/energies and reliance on low-cost, earth-abundant manganese (>50%). However, implementation of LMR materials is challenged by several issues such as voltage fade, hysteresis, and a rising impedance with cycling. Furthermore, fundamental understanding of the complex role of oxygen is still under investigation.

This presentation will discuss research and development efforts at Argonne National Laboratory, conducted under the Vehicle Technologies Office Cathode Consortium *"Earth-abundant Cathode Active Materials (EaCAM)"*, aimed at understanding some of the critical barriers to implementation of cobalt-free, LMR cathode-electrodes. Specifically, this presentation will present studies into the mechanisms of the anomalous impedance at low-states-of-charge as well as the overall impedance rise on extended cycling of LMR electrodes. A combined surface-treatment/electrolyte-additive has been used to help separate bulk vs surface behavior over long-term cycling. Connections to the correlated mechanisms of voltage fade and hysteresis will be discussed and a model describing impedance response presented.

12:40 PM

Na-Ion Delivery Via Molecular Cages in Porous Liquid Type-II Electrolytes

Sakshi Singh (University of Illinois Chicago)

Sodium-ion batteries are receiving more attention due to their low susceptibility to degradation by temperature change and having safety characteristics such as nonflammability. Further they are more cost effective compared to traditional Li^+ or Mg^{+2} batteries. Even so, they have limitation in commercialization mainly due to their low energy density, this is because of low mobility of Na+ ion. To address this challenge, we employ porous liquids, which exhibit high mobility with an ability to capture and carry Na+ ions. One of the porous liquids, crown ether type II (12C4) consists of an organic cage that can form a coordinate bond with Na+ ion and has high fluidity to transport and deliver ions and thus increasing the mobility of Na-ion. Here, we provide the mechanism of solvation, transport and electrical conductivity of the sodium ion through the porous liquid electrolyte. This study has the potential to improve the energy density of sodium ions in battery applications.

1:05 PM

Hybrid Air Conditioning Thermal Energy Storage for Space Cooling Applications

Said Al-Hallaj (University of Illinois Chicago)

Our group has developed a thermal energy storage system (TES) using composite phase change material (c-PCM) that was integrated in a Hybrid Air Conditioner (AC) + Thermal Energy Storage (TES) system. A commercial rooftop 5-ton air conditioning system was integrated with a 5-tonhr thermal energy storage and tested at the Thermal technology Facility at the National Renewable Energy Laboratory (NREL) in Golden, Colorado. The system proved concept viability and demonstrated a novel hybrid mode operation that reduces peak power draw and energy consumption, while minimizing total system cost.

The presentation will discuss data collected during the prototype unit testing at NREL including lessons learned and recommendations for further improvements. Namely, thermal transport characteristics in the composite phase change material as well as heat transport dynamics will be discussed. Additional improvements will be outlined to enhance charge/charge rates and prevent degradation of c-PCM material performance over time.

Session 1:
Track 2: Process Safety

Chair: Jessica Morris (Exponent)

Co-Chair: Nick Schulman (Exponent)

12:15 PM

Process Safety in Hydrogen Industries

William Giang (PSRG Inc.)

Hydrogen is a green and flexible source of energy. The world is moving toward a zero-emission future, it is increasingly clear that hydrogen fuel is an important energy substitution to combat climate change. Even though hydrogen production and safe handling is well-understood by the oil and gas industries, hydrogen safety in other sectors such as hydrogen fuel cells, electrolysis production, and the general public have not yet matured. As hydrogen's applications and demands increase, safe hydrogen production, transportation, and handling have become more important than ever. By implementing elements of Process Safety Management, knowledge can be transferred to the new industries to help better manage the hazard of hydrogen in their facilities.

12:40 PM

PSM Pillars…or Dominos? A Case Study to Consider the Link between Certain PSM Pillars.

Domingo Elias (Exponent)

OSHA's Process Safety Management (PSM) program provides a continuous, systematic approach to manage process safety. The PSM pillars have interdependency, and the effectiveness of the program is related to the implementation of the program pillars. Through examination of a case study, we will provide real-world examples of how breakdowns in one PSM element at a plant led to unintended issues with other PSM pillars-ultimately resulting in an observed incident at the plant.

The case study considered involves the replacement of a solenoid valve that supplies compressed air to a butterfly valve's actuator. Exponent investigated a plant that had replaced a 4-way solenoid with a 3-way solenoid valve, but the change did not trigger their MOC program. In this case, a leak of compressed air in the 3-way solenoid valve caused transient pressure spikes in the downstream pipeline due to fluttering (unintended oscillations of the butterfly valve's disc). These pressure spikes ultimately resulted in pipeline damage and leak of flammable hydrocarbon.

Because a 4-way solenoid valve and a 3-way solenoid valve are not "identical", the attempt to swap the valves should have likely triggered MOC. The systematic MOC process may have prevented the replacement of a 4-way valve with a 3-way valve or otherwise resulted in changes to the other impacted pillars of the PSM program: Process Hazard Analysis and Operating Procedures. In summary, we believe this case study provides useful real-world examples of how the lack of MOC can have unintended consequences to other PSM pillars and overall plant safety.

Session 2:
Track 1: Energy Storage II

Chair: Hakim Iddir (Argonne National Laboratory)
Co-Chair: Juan Garcia (Argonne National Laboratory)

1:45 PM

Structural Features in Li- and Mn- Rich Cathodes that Modify the Impedance at Low State of Charge

Juan Garcia (Argonne National Lab)

Lithium and manganese rich (LMR) oxides represent a viable option as a sustainable Li-ion battery cathode. Their advantages as affordable, energetically dense, and safe materials are well known. Their shortcomings, such as voltage fade and hysteresis, are also well known and they have been extensively studied. A less studied issue of LMR cathode materials is their high impedance at low states of charge (SOC). The high impedance is a limitation to using the full capacity of the LMR cathodes. Ab-Initio Molecular Dynamics (AIMD) simulations were used to understand the effect of distortions after activation in the composite materials. For the 60%-$LiMn_{0.5}Ni_{0.5}$/40%-Li_2MnO_3 composite material, AIMD show that the distortions of the lattice and the formation of oxygen dimers were confined to the well-delimited Li_2MnO_3 domains. The Mn-Ni 50/50 domains remained layered and undistorted after activation. AIMD calculated Li diffusivities show that Li mobility should be easier in the layered domains compared to the distorted Li_2MnO_3 domains. During discharge, the layered domains would be easy to fill first, and should manifest as a delayed onset of the impedance rise at low SOC. The AIMD simulation results suggest that high impedance can be attributed to the filling of Li_2MnO_3 domain Li sites. The composite material 60%-$LiMn_{0.5}Ni_{0.5}$/40%-Li_2MnO_3 with staggered domains presented uniform distortions of the lattice spread over the domains. Widespread but limited distortions would increase the impedance earlier in the lithiation process. Since in the staggered domains, there are no well-defined Li_2MnO_3 domains, the final impedance at low SOC is lower.

2:10 PM

Role of Crystal Size in Dynamic Charge Acceptance of Lead-Acid Batteries

Kevin Knehr (Argonne National Laboratory)

Lead acid batteries are important energy storage technologies used in a range of vehicle applications, including starting, auxiliary power, and micro-hybrid regenerative braking. A critical feature of lead acid batteries is dynamic charge acceptance (DCA), which is the ability to rapidly accept large amounts of charge. High DCA allows batteries to charge quickly, capitalizing on high powers from regenerative braking and ensuring the battery has ample charge to provide auxiliary services.[1] This work attempts to explain the influence of two factors on the DCA: the negative electrode carbon content and the previous cycle history. Increases in carbon content increase DCA.[2] Performing a DCA test (***e.g***, 2.4 V charge pulse from rest) after discharging the battery increases the DCA when compared to performing the test after charging, even if both tests are done at the same state of charge.[3] These relationships are investigated using mini electrochemical cells operated at different carbon contents and cycle history. The electrochemistry is analyzed using a model developed from porous electrode theory that includes a detailed description of the lead sulfate dissolution and lead plating kinetics at the negative electrode. Results suggest much of the behavior depends on the size distribution of the lead sulfate crystals within the porous electrode.

2:35 PM

Physics Informed Design of Porous Silicon-Based Electrodes

Abhas Deva (Argonne National Lab)

Over the last decade, silicon has become an increasingly attractive alternative to graphite as an anode material in lithium-ion batteries due to its low cost, low open circuit potential, and high specific capacity. However, large-scale commercialization has been plagued by the volume expansion that accompanies the lithiation and delithiation of silicon anodes, and its deleterious effects on battery life and cell design. This talk will present a thermodynamically consistent model, which combines electrochemistry with large deformation mechanics, to guide the design of silicon-based porous electrodes. The effect of electrode design parameters, such as thickness, porosity, particle size, etc., on the performance of silicon-based anodes will be discussed. Strategies to improve performance will be presented.

Session 2:
Track 2: Environmental Compliance/Remediation

Chair: Aditya Prajapati (LLNL)
Co-Chair: Taiwo Adesanya (UIC)

1:20 PM
Removal of Fluoride from Water Using Hybrid Aluminum-Magnesium-Calcium Coated Sand Adsorbent

Kiana Modaresahmadi (University of Illinois Chicago)

Fluoride contamination in natural water may occur due to the slow dissolution of fluoride minerals and their host rocks into groundwater as well as industrial discharges into waterways. The World Health Organization (WHO) recommends fluoride levels less than 1.5 mg/L in drinking water for prevention of major fluoride related health problems such as fluorosis, brain damage, thyroid disease, and cancer. Adsorption is a cost-effective technology for removal of fluoride from water in flow-through water filtration systems. Metal oxide adsorbents have the potential for effective removal of fluoride; among metal oxide adsorbents, aluminum oxide based adsorbents have shown promise as effective adsorbents of fluoride. In this study, an aluminum based three-metal oxide coated sand adsorbent was developed as a sustainable adsorbent for the adsorption and removal of fluoride from water with potential application in continuous flow adsorber systems. The hybrid aluminum-magnesium-calcium coated sand adsorbent was able to remove nearly 95 percent of fluoride from water with an initial concentration of 5 mg/L fluoride down to less than 1 mg/L fluoride. The removal of fluoride from water using the hybrid aluminum-magnesium-calcium coated sand adsorbent was evaluated as function of time, solution pH, adsorbent dosage, fluoride concentration and co-existing ions.

1:45 PM
Electrochemical Degradation of Perfluorooctanoic Acid Using Electrocatalytic Reactive Electrochemical Membranes

***Saurabh N. Misal* (University of Illinois Chicago)**

Electrochemical oxidation of concentrated perfluorooctanoic acid (PFOA) solutions that may be generated by ion exchange or foam fractionation was studied using Bi_2O_3, SnO_2, Bi-doped SnO_2 (BTO) and Pd deposited on a Ti_4O_7 reactive electrochemical membrane (REM). BTO was deposited on REMs using pulsed laser deposition (PLD) (BTO-PLD/REM), atomic layer deposition (BTO-ALD/REM), and electrodeposition followed by thermal oxidation (BTO-EDT/REM). Bi_2O_3, SnO_2 and Pd were deposited on REMs using ALD (Bi_2O_3-ALD/REM, SnO_2-ALD/REM and Pd-ALD/REM). Transmission electron microscopy analyses showed catalyst particle size ranging from 2.2 nm to 15.3 nm for the PLD method depending on the number of pulses used. By contrast, the EDT method produced much larger catalytic particles of ~ 1 micron in size. The electrodes fabricated by PLD and EDT deposition methods showed PFOA removal of > 92% of a 100 mM feed solution at an anode potential of 4.2 V/SHE and a residence time of ~11s, which was significantly higher than the Ti_4O_7 REM and other tested catalysts. The presence of Bi_2O_3 yielded higher fluoride compared to SnO_2 and Pd. The unbalanced fluoride was attributed adsorption of fluoride ions on REMs to F_2 formation. The formation of shorter chained perfluoroalkyl substances (PFAS) carboxylates with carbon chain lengths of five to seven was detected by the analysis of the treated solutions by liquid chromatography-tandem mass spectroscopy (LC-MS/MS). The detected products suggest a sequential CF_2 elimination mechanism during electrochemical oxidation. The experimental results were simulated by a reactive transport model, which suggests more than one mechanism could be involved.

2:10 PM
Electrochemical Reduction Using Ti4O7 Reactive Membranes Impregnated with Nickel and Iron for Pfas Destruction

Jacob King (University of Illinois Chicago)

Current PFAS treatment strategies generally employ adsorbents such as granular activated carbon or ion exchange to sequester these compounds from water. However, replacing spent sorbents can be complicated and costly. In addition, once sorbents are taken off-site for disposal, PFAS desorption kinetics are slow and their destruction is often incomplete, resulting in re-release of perfluorinated compounds into the environment. Recent oxidative and reductive technologies have demonstrated near complete destruction of PFAS, but oxidative processes frequently form undesired byproducts and reduction has primarily been done with hydrated electrons (e.g., via UV/sulfite), which require excessive energy inputs. Electrochemical reductive defluorination would be a lower cost alternative to advanced reduction processes that rely on hydrated electrons. The potential of transferred electrons can be adjusted, while electrode materials can be engineered to catalyze the transformation of PFAS. In the work presented herein, Ti_4O_7 reactive electrochemical membranes have been modified with nickel and iron to catalyze PFAS reduction. Voltammetry methods have been used to characterize reactivity of the electrodes with PFAS and initial bulk electrolysis results are presented.

2:35 PM

A Mechanistic Study on per-and Polyfluorinated Substances (PFAS) Electrooxidation on Ti4O7 Anode

Shirin Saffar Avval (University of Illinois Chicago)

Owing to their unique chemical and thermal stability, poly and perfluoroalkyl substances (PFAS) have been used extensively in different industries and products. This heavy use and recalcitrance have resulted in the accumulation of PFAS in the environment and detection in groundwater, wastewater, and landfill leachate. Furthermore, studies have shown that PFAS poses health risks, such as increasing the risk of cancer, thyroid problems, infertility, high cholesterol, and many more. Recent studies have focused on PFAS removal and destruction from wastewater. Electrooxidation is one process that shows promise for PFAS destruction. However, PFAS removal efficiency changes in the presence of different water constituents. To gain a better understanding of the PFAS oxidation mechanism, we have conducted a thorough investigation of the reaction of PFOA on a Ti_4O_7 electrode. A mechanistic understanding was accomplished through kinetic experiments, solution, and surface characterization techniques.

Session 3:
Track 1: Advances in Refining & Biorefining Technology

Chair: Rishabh Jain (Honeywell)
Co-Chair: Belma Demirel (bp)

3:15 PM

Life Cycle and Technoeconomic Analyses of Catalyst Used in the Conversion of Waste Plastic to Lubricate Oils from Upcycled Plastics (LOUPs)

Pahola Thathiana Benavides (Argonne National Lab)

Chemical recycling provides an alternative for plastic waste difficult recycling (i.e., films), as it breaks the polymer into chemical intermediates with high commercial value. Catalysts can play an important role in the deconstruction of waste polyolefin (PO) films into lubricating oils from upcycled plastics (LOUPs) with similar performance to conventional base oils and lubricants. Because catalysts can affect the economics and sustainability of these types of products, developing cost-effective and sustainable catalysts is key to achieving the economic and environmental viability of LOUPs. Despite their importance, catalysts are often simplified or even overlooked in techno-economic analysis (TEA) and life-cycle assessment (LCA) due to a lack of understanding and publicly available information. Therefore, in this work, we present the TEA and LCA of platinum strontium titanate (Pt/SrTiO3) catalyst used in the deconstruction of waste films to LOUPs. We discuss the process design of this catalyst by leveraging experimental results. The pre-commercial cost and environmental impacts are also estimated through models developed in ***CatCost*** and ***GREET*** (Greenhouse gases, Regulated Emissions, and Energy use in Technologies) tools funded by the U.S. Department of Energy. Preliminary estimates indicate a net catalyst cost of 585 USD per kg of catalyst, which is similar to other catalysts previously reported, and GHG emissions of 56 kgCO2e/kg of catalyst. The GHG are mainly derived from the use of solvents like ethanol and toluene. The outcomes of this study can help identify process stages in catalyst production with the potential to reduce costs and environmental impacts.

3:40 PM

Status of Blue H2 and Blue Ammonia As the New Decarbonized Fuel of Today and the Future

Jeron Chin (Haldor Topsoe)

Blue Hydrogen and Ammonia is leading the revolution as a fuel of the future by making a significant advances towards the decarbonization journey . The presentation will cover the latest developments and advances for large scale deployment of blue ammonia and hydrogen. The New Decarbonized Fuel Of Today And The Future – will be discussed.

4:05 PM

Effective and Efficient Chemical Recycling of Waste Plastics Is Dependent on the Presence of Catalysts

Jeff Martin (Ketjen)

The conversion of various waste streams into Waste Plastics Oil (WPO) requires upgrading regardless of the technology used or the waste being processed. Upgrading involves the removal of impurities, cracking of larger molecules, and/or saturation of double bonds to obtain the desired products. Therefore, hydrotreatment is typically necessary before feeding the WPO into a steam cracker or Fluid Catalytic Cracking reactor, or as a finishing step. Ketjen, with decades of experience in catalytic upgrading of crude oil fractions and renewable feedstocks via Hydroprocessing or FCC, is uniquely positioned to provide effective catalyst solutions for WPO upgrading and other renewable feedstocks.

The FCC unit is a flexible technology that can play an important role in achieving sustainable and circular objectives through the co-processing of renewable and waste-derived feedstocks. These feedstocks can include waste plastics, vegetable oils, and thermochemical oils produced from biogenic or waste-derived resources. Each feedstock presents its own advantages and challenges when co-processed in an FCC unit which can have a significant impact on the FCC process and catalyst requirements.

This presentation will highlight various catalytic solutions developed with our customers for renewables feeds and WPO upgrading. These solutions are based on case studies and collaborations with partners across the value chain. Examples range from catalyst systems required for co-processing WPO in existing refinery operations to the selective conversion of WPO into high-value chemicals. By combining an understanding of the required chemistry with a thorough knowledge of catalysts, the optimal catalyst system can be designed for each unique situation.

4:30 PM

Gas Fermentation: New Process Technology for a Circular Carbon Economy

Sean Rollag (LanzaTech)

Reaching the global net-zero carbon goals set by recent international agreements requires an all-encompassing approach that includes utilization of industrial waste carbon gas and recycling of solid waste carbon. LanzaTech's commercialized gas fermentation technology is an example of a novel process converting waste carbon emitted from an industrial process (steel production) into a platform molecule (ethanol). This platform ethanol can then be upgraded into jet fuel or consumer products (clothing, plastic bottles, etc.). Once these consumer products have reached the end of their lifetimes and become municipal solid waste (MSW), they can be recycled via gasification/fermentation into new consumer products, completing their carbon circle. This talk will discuss the progress and status of gas fermentation technology and LanzaTech's vision for a circular carbon economy.

Session 3:
Track 2: Green Engineering

Chair: Jason Wu (Honeywell UOP)
Co-Chair: Omar Aly (UIC)

3:15 PM

Computational Screening of MOF and Working Fluid Pairs for Adsorption Cooling Applications

Filip Formalik (Northwestern)

The use of adsorption cooling systems has gained significant attention in recent years due to its potential to provide energy-efficient and environmentally friendly cooling solutions. Metal-organic frameworks (MOFs) have emerged as a promising class of porous materials for adsorption cooling applications. These materials have highly tunable porous structures, which can be tailored to this specific application by varying the metal ions and organic linkers used in their synthesis. Our study aimed to identify the most promising MOF + fluid pairs for use in these systems using molecular simulations. We employed grand canonical Monte Carlo (GCMC) simulations to examine the adsorption of propane and isobutane in various MOFs. These alkanes were recommended by the U.S. Environmental Protection Agency as substitutes for chlorofluorocarbon and hydrochlorofluorocarbon as a green choice in household and retail food refrigerators to reduce ozone layer depletion. High-throughput GCMC simulations allowed us to screen over 400 MOFs to identify the best-performing subset. Our simulations revealed that MOFs exhibited promising adsorption cooling properties for both fluids. Additionally, we compared their performance with previously reported frameworks and other adsorbents such as activated carbon or zeolites and found that some MOFs can reach a significantly higher cooling capacity compared to any material considered to date. This research provides a valuable step toward the identification of suitable MOF + fluid pairs for green adsorption cooling applications. Further research is necessary to confirm the simulated results experimentally and optimize the structural and chemical properties of the frameworks to maximize their performance.

3:40 PM

Graph Neural Network Model to Predict Carbon Adsorption Capability of MOF

Hyun Park (University of Illinois Chicago)

Finding metal organic frameworks (MOF) with high CO2 adsorption capability is of great interest for industrial and commercial applications. However, computing CO2 adsorption capability of MOF with conventional simulation approaches such as molecular dynamics (MD) or monte carlo (MC) can be computationally costly. This slow and costly process can be a bottleneck in searching for high-performing MOFs. With the assistance of machine learning (ML) methods, we can speed up search for the high-performing MOF candidates. In this work, we propose use of graph neural network (GNN), which takes atomic coordinates of a MOF as input, to predict CO2 adsorption capability. GNN, unlike conventional ML methods such as decision tree, does not need manual data-preprocessing to use as feature input. Also, we redesign GNN models such as CGCNN to both boost training speed and to increase CO2 adsorption prediction accuracy with faster convergence. Lastly, we show that GNN can provide ML insight of how CO2 adsorption capacity is predicted via analyzing GNN’s learned data representation. In conclusion, our work requires no data-preprocessing and yields high accuracy property prediction at less computational cost, with added benefits of understanding what ML model has learned.

4:05 PM

Diffusion Model Accelerates Computational Design of MOF Structures for Carbon Capture

Ruijie Zhu (Northwestern)

The modular nature of metal-organic frameworks (MOFs) allows for property tuning by varying the types of building blocks and their connectivity. For carbon capture applications, MOF linkers have been shown to determine key geometrical features and adsorption properties. We propose an iterative isoreticular design framework for generating new MOF structures with improved CO_2 working capacities. This framework adopts a deep learning-based diffusion model DiffLinker to generate new linkers, which are assembled into MOFs with pre-selected nodes in a given topology. By varying the number of atoms sampled between two or more molecular fragments, the diffusion model enables efficient generation of 3D coordinates of new linkers. A modified CGCNN model is then used to predict the CO_2 working capacities of the assembled MOFs. We demonstrate the utility of our framework on the open source hMOF dataset, where we compare the generated linkers with existing ones parsed from hMOF dataset using metrics such as novelty and uniqueness. We prioritize linkers with lower synthetic complexity when screening. This framework has been deployed on the ThetaGPU supercomputer to accelerate the search for MOFs with high CO_2 working capacities at a given pressure. The structural features of low and high performers are analyzed, and the best performers are suggested for experimental synthesis.

4:30 PM

Left or Right? Which Way on a Decarbonization Journey?

Katelyn Tran (Wood Group USA)

The race to net-zero and/or a low carbon status quo is rapidly accelerating across all sectors of the global economy. Global corporations are re-aligning their organizations to tackle their business challenges to meet climate change commitments. In the United States, with the most recent US inflation act, hard-to-abate industrial sectors such as LNG, refining, petrochemical, steel, cement, and others are perceiving an improved economic environment to justify and implement decarbonization solutions to their operations. Among various decarbonization solutions, two show the most promising advantages for industrial scale application: 1) Hydrogen as fuel source and 2) Carbon Capture.

In this paper, a case study is presented using a typical large refinery facility located in the United States Gulf Coast region and compares the technical and economic aspects of using Hydrogen as a fuel source, fully or partially, versus implementing Carbon Capture.

The sample refinery facility used in this study processes more than 600,000 barrels of oil per day, including power generation facilities (>1,000 MW), consuming either natural gas, refinery fuel gas or a mix; and emits a total of more than 7.0 million metrics tons per year of CO2.

Findings of this study suggest that the decision to go "left" or "right" in this decarbonization journey go beyond the simple comparison of the CO2 abatement costs. Full engagement with owners/operators of facilities like these ones is imperative to fully align technical, operability, economic and sustainability goals. Corporations would need to travel both roads to arrive to the same destination

Local Section Dinner and Dinner Keynote

7:00PM Keynote

The Consumer Case for Electric Vehicles

Quinta Warren (Consumer Reports)

Electric vehicles (EVs) have zero tailpipe emissions, so they are an excellent technology for reducing both GHG emissions and air pollution from transportation. They also save consumers money on fueling and maintenance costs as they are more efficient than internal combustion engine vehicles.

Consumer Reports' surveys and analyses show that a growing number of Americans are interested in EVs. Yet, barriers persist that prevent greater adoption of these vehicles, including in overburdened communities. I will discuss what role government, manufacturers, and advocacy organizations like CR can play to help consumers overcome these barriers and speed up the transition to cleaner transportation.

Presentation Abstracts (Day 2)

Wednesday, April 12, 2023

Session 1:
Track 1: Bioengineering & Nanotechnologies

Chair: Meltem Urgun-Demirtas (Argonne National Lab)

9:00 AM
INSERT TITLE

INSERT ABSTRACT

9:25 AM
Will Future Generations of N95 Masks Include Atomic Layer Deposited Silver Nano-Islands?
Harshdeep Bhatia (University of Illinois Chicago)

Due to the COVID19 outbreak, there has been increasing interest in tailoring, modifying and improving conventional personal protective equipment to increase their service life and make them more effective against viruses and bacteria. Previously, Ag nanoparticles have been successfully immobilized on fibers and other mask materials. However, in this study, ALD was used to grow Ag on N95 masks in the form of nano-islands. This was done to ensure the Silver does not detach or leach into the air since nano-islands are known to be chemically stable. In this study, ALD reactions were performed using a custom-built reactor on N95 mask using a silver precursor along with a reducing agent. X-ray photoelectron spectroscopy and x-ray absorption fine structure were used for silver ALD characterization; microbiological assay was conducted to study the effectiveness of the deposited silver against the air-borne pathogen ***Staphylococcus aureus (S. aureus)***. The leaching of silver nano-islands was studied using inductively coupled plasma mass spectrometry of phosphate-buffered saline (PBS) solution after soaking the mask in it over predetermined times. Results showed that the layers of N95 mask were successfully functionalized using silver ALD. The deposited silver nano-islands were stable on the N95 filter media against washing. Antimicrobial properties were observed on the deposited mask. This opens doors to not only functionalizing N95 masks but other fibers that contain silver to replenish and significantly enhance their antimicrobial activity.

9:50 AM
Developing a Platform for Induced Pluripotent Stem Cell Reprogramming through Lipid Nanoparticle Based mRNA Delivery
Emily Kim (UPenn*)*

Induced pluripotent stem cells (iPSCs) are derived from adult somatic cells and have shown potential in regenerative medicine since they have the potential to differentiate into a multitude of cell types without the controversial use of embryos. However, iPSCs are difficult to transfect. The most common transfection methods are lipofection and electroporation, but the methods have low efficiency and a high death rate. One potential transfection method is utilizing lipid nanoparticles (LNPs), which are drug delivery vehicles that can have a wide multitude of cargo such as mRNA and siRNA. LNPs have already been FDA-approved for COVID-19 vaccines as a method to deliver mRNA. They also have high transfection potential in iPSCs, but they must be optimized for specific applications since the formulations are not universal. In this project, we screened various LNP formulations with lipids with different characteristics. We evaluated both branched and unbranched lipids in addition to lipids of varying tail lengths for their transfection efficiency in iPSCs. Several dose responses were performed in iPSCs to evaluate toxicity and transfection efficiency. The results indicated that branched lipids consistently performed better than linear lipids, and we have identified a lead LNP candidate that can transfect iPSCs at a wide range of doses with minimal toxicity. We plan to use this lead candidate to reprogram iPSCs using CRISPR/Cas9 in *ex vivo* therapy.

Session 1:

Track 2: Machine Learning & Optimization

Chair: Aashutosh Mistry (Argonne National Lab)

9:00 AM

Hybrid Series and Parallel All-Nonlinear Dynamic Static Neural Networks: Development, Training, and Application to Chemical Processes

Angan Mukherjee (WVU)

Developing accurate first-principles models for nonlinear dynamic systems can be computationally expensive. Data-driven models are relatively easier to develop but have their disadvantages in accurately representing nonlinear systems. For many nonlinear dynamic systems, it can be difficult to adequately model them using a simple standalone static, dynamic or linear-time-invariant dynamic model integrated with a nonlinear static neural network, without suffering from the curse of dimensionality. Therefore, it is desired to consider both static and dynamic models to be nonlinear, thus making it challenging to synthesize optimal hybrid networks. This work proposes efficient algorithms for training hybrid series and parallel static-dynamic networks with nonlinearities in both static and dynamic models.

Conventional backpropagation algorithms may require significant tuning of hyper-parameters and suffer from slow convergence. Furthermore, the best optimization algorithm for converging the static model may be different than that for the dynamic model. This work focuses on developing sequential algorithms for hybrid networks where the static and dynamic networks can be trained independently by different optimization algorithms, with an outer layer optimization for estimating the connection weights between them. The developed algorithms are flexible for incorporating modifications in network architecture and including constraints. Both series and parallel architectures have been considered to develop models that offer tradeoff between computational expense and accuracy.

The proposed algorithms are applied to model three nonlinear dynamic processes, including a pilot-plant for post-combustion CO_2 capture. The proposed hybrid all-nonlinear series and parallel models show superior performance compared to prominent state-of-the-art models like LSTMs, GRUs, and DABNet.

9:25 AM

Accelerating MOF Synthesis Via Data Mining and Machine Learning

Manuel Tsotsals (Karlsruhe Institute of Technology)

The chemical space of metal–organic framework (MOF) materials offers an almost infinite space of compositions, structures, properties, and applications. [1-2] Computer-assisted methods have been applied to for the discovery [3-4] and the modification [5] of MOF. However, the potential of using machine learning (ML) methods to suggest parameters in MOF synthesis experiments is not well explored. In this study, we demonstrate how data mining and machine learning can be employed to rationalize and accelerate the MOF discovery process by directly predicting the synthesis conditions of new MOF materials based on their crystal structures. Our approach contains three distinct steps: 1) The creation of a MOF synthesis database (SynMOF) through automated extraction of synthesis parameters from scientific literature, 2) The training of multiple ML models on the SynMOF database, and 3) The prediction of synthesis conditions for new MOF structures through the use of our ML models. These early-stage ML models surpass the predictions of human experts, as evidenced by a synthesis survey taken by international MOF synthesis experts.

9:50 AM

Small Molecule Adsorption Energy Predictions for High-Throughput Screening of Electrocatalysts

Srishyam Raghavan (University of Illinois Chicago)

Predicting adsorption energies of small molecules (e.g., OH, and OOH) on electrocatalysts involved in electrochemical reactions aids in accelerating the design and screening of electrocatalysts. Avoiding computationally expensive electronic structure calculations increases the speed of such predictions. Geometric and electronic descriptors have been reported to characterize the environment around surface active sites and predict adsorption energies. However, these descriptors cannot be used to predict adsorption energies of small molecules on various substrates, e.g., metal oxide and nonmetal electrocatalysts. We compare the performance of these descriptors in predicting adsorption energies of small molecules on various electrocatalysts with adsorption energies from density functional theory calculations. We show that two recently developed machine learning algorithms, Crystal Graph Convolutional Neural Network (CGCNN) and Atomistic Line Graph Neural Network (ALIGNN) outperform the reported geometric and electronic descriptors in predicting the adsorption energies. Our results suggest that ALIGNN is almost always more accurate than CGCNN in adsorption energy predictions. The improvement ranges from 0.02 to 1 eV in the mean absolute errors (MAEs). We also compare the performance of CGCNN and ALIGNN algorithms in predicting the overpotentials of the oxygen evolution reaction occurring on various electrocatalysts with MAEs of 0.06 and 0.05 V, respectively.

Session 2:

Track 1: Bioengineering & Nanotechnologies

Chair: Meltem Urgun-Demirtas (Argonne National Lab)

10:30 AM

Inter-Electronic and Inter-Valley Transitions in MoS2 WS2 Heterostructures and Alloys

Sungjoon Kim (University of Illinois Chicago)

Van der Waals heterostructures allow the integration of functionalities from different nanomaterials to obtain enhanced superimposed properties, or entirely new physical properties. In this study, vertical and horizontal MoS_2-WS_2 heterostructure grains were grown using atmospheric pressure chemical vapor deposition, and their optoelectronic properties were investigated. The field effect transistors fabricated from the heterostructure grains exhibited high photoresponsivity, which was influenced by the gating potential, as well as the measurement temperature. During the gating potential sweep from -5 V to +55 V, the light to dark source drain current ratio (I_{light}/I_{dark}) increased from 3 to 16 and from 2 to 7 at 60 K and 120 K, respectively. Alloy of $Mo_xW_{1-x}S_2$ grains were also obtained, which displayed valley coherence when irradiated with linearly polarized light. The degree of valley coherence was approximately 49% at room temperature. Such phenomena can be leveraged to realize novel optoelectronics, computing, and memory applications.

10:55 AM

Tunable Sulfur Incorporation into Atomic Layer Deposition Films Using Solution Anion Exchange

*Julia Lenef (*University of Michigan)

Atomic layer deposition (ALD) is a powerful technique to fabricate metal sulfide and oxysulfide films, which can be used as functional materials in solar cells, catalysts, and electronic devices. Although ALD of sulfur-containing materials provides precise control of thickness, composition, and high uniformity on 3D architectures, it typically uses H_2S—a toxic, corrosive, and flammable gas—as the sulfur source. To address these safety challenges, we developed a process to incorporate sulfur into ALD metal oxide films using a solution sulfur anion-exchange process, which does not rely on H_2S gas.

CuO_x (i.e. CuO and Cu_2O) deposited by ALD is chosen as a model system to investigate the effect of anion-exchange chemistry in aqueous conditions. We show that the sulfur content in the ALD CuO_x films can be controlled by varying the reaction time, solution molarity, and temperature. The temporal evolution of sulfur incorporation can be described using a coupled reaction-diffusion model. Changes in composition, crystal structure, and morphology observed during anion exchange were quantified by X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), and atomic force microscopy (AFM). Conformal sulfur incorporation was achieved on a core-shell nanowire, providing evidence that the conformality of the initial ALD process can be maintained during anion-exchange on high-aspect-ratio structures. To illustrate a pathway towards device fabrication, area-selective sulfur anion-exchange was realized on micro-patterned substrates by photolithographic patterning. Finally, the electrical properties were evaluated, indicating a tunable reduction in sheet resistance of up to four orders of magnitude as sulfur is incorporated in the CuO_x films.

Session 2:
Track 2: Machine Learning & Optimization

Chair: Aashutosh Mistry (LLNL)

10:30 AM

Generative Adversarial Network to Accelerate Computational Screening of Metal-Organic Framework Structures

Xiaoli Yan (University of Illinois Chicago)

The challenge of designing novel metal-organic framework (MOF) structures with desired application performances lies in the chemical compositions' finite but vast search space. This search space usually consists of a constant list of metal secondary building units (SBU), organic linkers, and topologies. Although the combinations of the building blocks are finite, all combinations require tremendous computational and experimental effort to screen through. Many machine-learning models have been applied in this area to reduce the number of simulations and experiments. Generative machine learning models are designed to generate candidates while learning the pattern of the training inputs. In this work, we propose a generative adversarial network (GAN) model to aid the design of MOF structures. This GAN model can not only generate new combinations of building blocks for the MOF structures, but the building blocks within each new combination can also be new. The assembled MOF structures from the combinations of building blocks are checked for uniqueness, chemical validity, and application performances. A quantitative metric is assigned to each MOF structure that passed the evaluation, and the generator of the GAN model is further optimized to suggest better building blocks and combinations in the next round. This closed-loop workflow can be run continuously to provide candidates with a higher success rate for the computational and experimental efforts. All data used in this study are from open-access databases, and all software libraries used in this study are open-source.

10:55 AM

Exploring MOF Sorption Properties with Topological Data Analysis

Seth Moore (University of Chicago)

We use Topological Data Analysis (TDA) to diagnose correlations between the geometric features of Metal-Organic Framework (MOF) composition and its expected CO_2 working capacity, predicted from Grand Canonical Monte Carlo molecular simulation. TDA encodes the periodic geometry of the unit cell by numerically projecting how the atomistic connectivity changes over some user-defined distance metric. This topological projection is represented via persistence diagrams that outline porous surfaces and volumes as 1 and 2-dimensional holes, respectively. Our TDA-based methodology shows significant advantages to binary or categorical metrics because it allows more robust comparisons between different crystal structures and their topologies, determined by their node-linker geometries. We show a statistical correlation between MOFs with pore diameters between 9-11 Angstroms and above-average working capacity in the hMOF dataset. Finally, we discuss how this form of topological featurization can be used in conjunction with regression and generative models.

Wednesday Afternoon Keynote Session

12:55 PM

Integrating Multiscale Modeling and Optimization for Sustainable Process Development

Frank (Xin) Zhu, Lijun Xu (Honeywell UOP)

The new approach for process development discussed in this presentation is based on integrated molecular modeling, process integration and mathematical optimization. By incorporating fundamentals into process development, it can identify the best molecular transformation routes by optimizing reaction pathways. Furthermore, mechanistic kinetic modeling such as microkinetic modeling and molecular-based kinetic Monte Carlo, which is enhanced by quantum chemistry, can help predict yield selectivity incorporating catalyst properties and structures for deriving different catalyst formula. Process integration is about selecting fit-for-purpose technologies for reaction, separation, and heat transfer systems, while mathematical optimization is about obtaining the optimal process flowsheeting and conditions to achieve the desired products with the lowest capital and operating costs as well as minimal footprint such as plot space, various emissions and wastes, hydrogen, water, and energy. By mathematical optimization based on fundamental models and process integration options, it can identify technological breakthrough ideas. For given multiple objective functions, mathematical combinatory optimization of the fundamental models not only determines the best-fit technology profile for an overall process based on techno-economic criteria, but also allow the process to deal with different feedstocks and make product shift based on market needs as well as the best environmental performance.

Session 3:

Track 1: Catalysis I

Chair: Trevor Lardinois (Exponent)

Co-Chair: Nicole Libretto (Honeywell)

2:00 PM

Amino Acid Glycine-Derived Metal-Free Nitrogen Doped Ordered Mesoporous Carbon for Efficient Electrochemical Synthesis of Hydrogen Peroxide (H2O2)

Basil Rawah (Illinois State University)

Electrocatalytic partial oxygen reduction has been considered a more sustainable approach to the synthesis of hydrogen peroxide (H_2O_2), as compared with current industrial anthraquinone processes. One key research need is to explore low-cost active electrocatalysts. Here, we report a facile, solvent-free method to synthesize a metal-free nitrogen-doped ordered mesoporous carbon (N-OMC) by in situ transforming of glycine (carbon and nitrogen precursors) in the mesoporous SiO_2 template (KIT-6) followed by subsequent thermal treatment at different temperatures. Among all samples, the catalyst treated at 800 °C (N-OMC-800), the nitrogen-rich carbon, exhibits outstanding structural properties and porosity, showing the dominant formation of pyrrolic-N and graphitic-N. With combined improved structural properties with the optimal ratio of N-pyrrolic/N-graphitic, P/G carbon provided an outstanding electrocatalytic activity, promoting H_2O_2 with high selectivity and production rate in alkaline mediums. The N-OMC-800 can achieve a faradaic efficiency (FE) of ~100% to H_2O_2 at (0.6 V_{RHE} to 0.4 V_{RHE}) in a H-cell containing 0.1 M KOH. Furthermore, its bulk H_2O_2 electrosynthesis in our self-designed flow cell confirmed its practical capability by showing a remarkable H_2O_2 production rate of 9.43 mol gcat^{-1} h^{-1} at 0.35 V_{RHE} and maintaining nearly 100% FE at the cathode potential of 0.6 V_{RHE} for 12 h without any degradation.

2:25 PM

Ligand-Coordination Effects on the Selective Hydrogenation of Acetylene in Single-Site Pd-Ligand Supported Catalysts

Eman Wasim (Indiana University)

Single-atom catalysts have the potential to achieve high levels of selectivity in heterogeneous catalysts. We have applied a metal-ligand strategy to create single-atom Pd catalysts on CeO_2 supports for the partial hydrogenation of acetylene to ethylene. Ethylene is a vital raw material with increasing global demand in the polymer, pharmaceutical and petroleum industries. Typically, ethylene is produced by the steam cracking of naphtha. The product stream from the steam cracking of naphtha contains ethylene and propylene along with a small concentration of unsaturated hydrocarbons. Effective ethylene polymerization requires that the ethylene feed stream contain minimal acetylene to avoid poisoning the polymerization catalyst. Our group has developed highly selective single-site catalysts using a metal-ligand coordination strategy by complexation of Pd with the ligand 1,10-phenanthroline-5,6-dione (PDO) on cerium oxide powder supports. In this presentation, we design on-surface metal-organic complexation, which acts to bridge the gap between homogeneous and heterogeneous catalysis, and provides metal sites on powder oxide supports that are active and selective for hydrogenation of acetylene to ethylene. In this joint experimental and theoretical investigation, the effect of organic ligand and its impact on the activity, selectivity, and stability of supported single-atom Pd metal is examined. In the metal-ligand approach employed, the supported metal species form Pd-ligand single-atom catalysts (SAC) on pristine powder supports. The activity of these catalysts shows a significant dependence on the choice of ligand and type of support. Understanding the support-metal interaction is crucial to advance the design of highly dispersed single-site catalysts for heterogeneous reactions.

2:50 PM

First-Principles Analysis of the Ammonia Decomposition Reaction on High Entropy Alloy Catalysts

Zuhal Cakir (Purdue University)

The development of periodic Density Functional Theory (DFT) calculations, combined with advanced synthesis techniques, has accelerated the understanding and development of multimetallic alloy catalysts. Recently, a new class of materials, high entropy alloys (HEAs), has opened up additional catalyst design possibilities in the alloy space. HEAs are comprised of many principal elements, with completely mixed atomic structures, leading to potentially millions of unique chemical environments around active sites. These materials have attractive properties for catalysis, including enhanced stability due to entropic effects, as well as highly tunable active site structures that could be exploited to optimize catalytic activity and selectivity.

In this study, we systematically develop a model of high entropy alloy catalysts, randomly-ordered bimetallic alloys, and extend these ideas to incorporate multiple elements. We develop tools to efficiently sample different binding sites and to investigate the free energy landscape for simple adsorbates on these sampled sites. To illustrate this approach, we choose the ammonia decomposition reaction as a probe reaction and Co-Mo as a model catalyst, based on the promising activity demonstrated experimentally for this chemistry on Co-Mo-based HEA's. We determine the binding energies of various reaction intermediates on many randomly sampled arrangements of the HEA surfaces using DFT. We deduce that the rate-determining step for the ammonia decomposition reaction is recombinative nitrogen desorption. This conclusion remains constant across the different considered surface arrangements. The results form a strong basis for further studies and the development of high entropy alloy catalysts for ammonia decomposition.

Session 3:
Track 2: Fluid Properties, Fluid Dynamics, & Transport Phenomena

Chair: Hadjira Iddir (Honeywell)

2:00 PM

Performance of a CSTR Activated Sludge with Different Configurations for Municipal Wastewater Treatment

Seyed Amirfakhri (University of Wisconsin)

Four activated sludge (AS) units with CSTR aeration tank and different configurations of feed, return sludge, and internal recycle streams are simulated in Mathematica using the activated sludge model No.3 (ASM3). The AS units include an anoxic tank, ideal CSTR aeration tank, and ideal clarifier. Conventional AS, AS with internal recycle stream from aerobic to anoxic tank, AS with step feeding, and AS with return sludge to both anoxic and aerobic tanks are studied under identical operating conditions. A wastewater stream with a flow rate of 1000m^3/d, total COD of 279g/m^3, and ammonia concentration of 12.5g/m^3 enters the AS units. All configurations work under identical operating conditions. The units are simulated in Mathematica and removal efficiency of slowly biodegradable substrates, readily biodegradable substrates, and ammonia are determined. Moreover, nitrate concentration in the effluent of the units, SRT, sludge production rate and air flow are calculated. This information will be used to compare the performance of these units for COD removal, nitrification, and denitrification. The results indicate that the unit with return sludge to both anoxic and aerobic tanks presents the maximum removal efficiency of COD and requires the maximum air flow rate. This unit has the minimum sludge production rate. The unit with internal recycle stream presents superior performance for denitrification and requires the minimum air flow rate.

2:25 PM

Obtaining Structural Information of Carbon Black in Carbon Black/Polyvinylidene Difluoride Suspensions with Simultaneous Rheo-Electric Measurements

Qingsong Liu (Northwestern)

Lithium-ion battery slurry containing carbon black has a microstructure that depends sensitively on how it is processed due to carbon black's (CB) evolving structure when subjected to shear deformation. While polymer binder polyvinylidene difluoride (PVDF), one of the main components of the slurry, plays an important role in modifying the structure and the rheology of CB, a quantitative understanding of the polymer role under shear is lacking. We used rheo-electric measurements to show that the addition of PVDF modifies the structure of CB agglomerates through the indirect effect on the solvent viscosity. Simultaneous impedance measurements were conducted on these CB/PVDF suspensions in shear flow as a function of carbon and PVDF composition. We found that the CB agglomerate size information can be derived from normalized suspension viscosity through rheological measurements. Additionally, the further validation of such size information is evident in the dielectric strength of the relaxation process obtained from impedance measurements. These findings will be valuable to energy storage systems containing CB as the dispersion of CB can be predicted and controlled with tunable processing conditions to optimize the performance.

2:50 PM

Modeling and Numerical Simulation of Concentrated Solar Energy Storage in a Packed Bed of Silicon Carbide Particles

Zeyuan Gao (Illinois Institute of Technology*)*

A radiative heat transfer model is developed, and a computational fluid dynamics (CFD) approach is used to simulate concentrated solar energy (CSE) storage by a packed bed of silicon carbide (SiC). Radiative heat transfer plays a very important role when the temperature is high, such as the temperature of a medium upon receiving radiative CSE. In this study, the radiative heat transfer in our packed bed was modeled as an effective conductivity based on the Breitbach and Barthels study. We considered a two-dimensional model and ANSYS Fluent 16.1 was used to conduct our numerical simulations. The result of our two-dimensional simulation agreed well with the temperature measurements of SiC particles in a packed bed by Tregambi et al. The effects of the airflow and radiative energy flux distribution on the packed bed energy absorption were simulated. An increase in energy absorption was calculated using wider radiative energy flux distribution. Our numerical simulations showed that a packed bed system with lower bed height and larger cross-sectional areas to accommodate wider multiple distributions of incident energy sources significantly enhances the capacity of CSE energy storage using a packed bed system. Furthermore, our numerical simulations showed that a packed bed with an optical quartz tube where the radiative energy meets the surface of the packed bed results in more widely distributed concentrated solar energy on the tube surface and an increase in energy absorption and storage capacity.

Session 4:

Track 1: Catalysis II

Chair: Nicole Libretto (Honeywell)
Co-Chair: Trevor Lardinois (Exponent)

3:30 PM
Mechanistic Insight into Tris(pentafluorophenyl)Borane Speciation during Ring Opening of Epoxides
Hiyab Mekonnen (Northwestern University)

Epoxide ring opening is an important route to 1,2-difunctional organic compounds, and it is essential in the production of polyether polyols used in the polyurethane industry. The ring opening of epoxides by alcohols produces either the primary (P1) or secondary (P2) alcohol regioisomer. In the polyurethane industry, there is a demand for selectivity towards primary polyols (e.g. P1) derived from propylene oxide, as polyols terminated in secondary alcohols result in poor reactivity and disrupt the humidity resistance. Unlike most commercially available catalysts, tris(pentafluorophenyl)borane (BCF) is a strong molecular Lewis acid catalyst that favors the formation of P1 over P2. During the ring opening of epoxides by alcohols, evidence indicates that BCF proceeds not only through a Lewis acidic pathway, but also through water and alcohol mediated pathways, depending on the extent of reaction, the alcohol nucleophile, and reaction conditions. We seek to extend these models to higher temperatures and lower catalyst loadings where catalyst deactivation and side reactions become more significant, and we seek to provide direct evidence for some of the proposed catalytic species. Here, we combine experimental results from variable temperature NMR with density functional theory (DFT) calculations and microkinetic modelling to get insights on the kinetics and deactivation mechanisms.

3:55 PM
Non-Thermal Plasma Assisted Catalytic Water Splitting for Clean Hydrogen Production at Near Ambient Conditions
Mingyuan Cao (Notre Dame)

The catalytic non-thermal plasma (NTP) reactors have been widely applied for various plasma-assisted reactions to improve performance owing to the existence of the synergistic effect between plasma and catalyst. Herein, for the first time, the catalytic NTP reactors were engaged for hydrogen production by water splitting to explore the catalyst role in performance improvement. A preliminary catalyst, Au/(TiO_2/SBA-15) (SBA-15: Santa Barbara Amorphous-15), was used to conduct catalyst optimization by adjusting metal loading amount, TiO_2 loading amount, catalyst support type and metal species. The optimized catalyst was with a formula of 0.2 wt.% Au/(10wt.% TiO_2/SBA-15) and its hydrogen production rate was high up to 1.03 mL min^{-1} with a 36.9% water conversion,which is 245% of the performance of the NTP reactor without catalyst packing. To explore the inherent factors affecting the catalyst performance, the surface properties of the catalysts, such as specific surface area, pore volume and water adsorption amount, were investigated and correlated with the catalyst performance. Based on these, a hypothetic reaction mechanism that emphasizes the importance of surface discharge is proposed and a catalyst design principle is drawn as a catalyst with large surface area and pore volume as well as a moderate H_2O adsorption amount performs the best. In theory, chemical kinetics modelling of H_2O/Ar plasma was conducted to figure out possible reaction pathways for hydrogen production. The application of catalyst in NTP-assisted water splitting presents a promising path for performance promotion.

4:20 PM
Deciphering Activity Controls for Ethylene Oligomerization Catalyzed By Metal Ions Grafted on

Oxide Supports By Computational Interrogation

Neha Mehra (Notre Dame)

Group-4 metals (M^{4+} = Zr, Ti, Hf) anchored on silica and silica-alumina are reported to be active catalysts for ethylene coupling and hydrogenolysis of paraffins to fuel range hydrocarbons. Density functional theory (DFT) calculations are employed to rationalize their observed activity. We construct atomistic models of metal sites grafted on (111) surface of ß-cristobalite, a silica polymorph. While Group-4 ions are isovalently substituted into silica, substitution of Al^{3+} produces more diversity into the reactive site with the introduction of proximal BrØnsted and Lewis acidic sites. We contrast ethylene oligomerization and hydrogenolysis pathways for Group-4 ions on silica and Al-doped silica to probe the synergistic effect of different acid sites on reaction pathways, including Cossee-Arlman chain growth and ß-termination mechanisms. Microkinetic models parameterized on DFT-based rate constants are applied to infer reactivity under experimental conditions and compare predictions with observations. Degree of rate control analysis shows that the steps controlling the rates vary across these sites. The approach is extended to examine the role of charge and of partially filled d-orbitals on reaction pathways for similarly constructed Ga^{3+}, Zn^{2+}, Ni^{2+}, Co^{2+} sites on silica. Results obtained aid in understanding trends across metal ions and factors governing their activity towards hydrocarbon conversion reactions relevant to today's economy based on oil and increasing production of shale gas.

Session 4:
Track 2: Polymers

Chair: Carina Martinez (U Chicago)
Co-Chair: Cheryl Slykas (UIC)

3:30 PM

Molecular-Level Insights into the Diffusion Mechanism of a Hydrophobic Drug from a Block Copolymer Micelle By Molecular Dynamics Simulation

Negin Razavilar (Kettering University)

Previously, all-atom molecular dynamics (MD) simulations of a single hydrophobic drug molecule in a series of poly (ethylene oxide-b-caprolactone) (PEO-b-PCL) pseudo-micelles were performed to gain insight into the drug-polymer interactions and drug diffusion. Although some insights into the hydrogen-bonding interactions could be obtained from these simulations, it was not possible to capture the full effect of the interactions on the drug diffusion dynamics. All-atom MD simulations of drug diffusion from stable drug-loaded micelles are prohibitively costly due to the very long timescales associated with drug release from such systems. To reduce the computational cost, in this study, we performed an all-atom MD simulation starting from a *disordered* structure of a full Cucurbitacin B (CuB)-loaded PEO-b-PCL block copolymer micelle in water. We found that the ensuing drug diffusion out of the micelle is mediated first by the formation of water-PCL bonds and breaking of water-PEO bonds, and then by the formation of water-CuB bonds. The CuB and water dynamics yielded nonlinear sub-diffusive mean-squared displacements, owing to the molecular crowding in the micelle and hydrogen bonding interactions between the water/CuB molecules and polymer chains. Finally, we found that the hydrogen bonding and diffusion dynamics in the pseudo-micelle are not representative of those in the full micelle. The computational approach used in this study is expected to yield molecular-level information that can aid in understanding in-vitro drug release data from nano-sized polymer micelles.

3:55 PM

Upcycling Virgin and Waste Polyethylene to Reprocessable Dynamic Covalent Networks Via Free Radical Grafting of Dialkylamino Disulfide Bonds

Logan Fenimore (Northwestern))

Plastics enable modern life through their advantageous properties and broad applicability. Regardless of their type or use, plastics are challenging to recycle efficiently. Current methods for recycling spent thermoplastics such as re-extrusion with additives result in property degradation over time and the relegation of these downcycled polymers to low-value applications. Plastics may be permanently cross-linked into thermosets, yet permanent cross-links prevent these plastics from being processed and molded into new shapes at high temperature. An emerging avenue to mitigate these sustainability problems involves enriching waste plastics with dynamic covalent bonds as chemical cross-links. By introducing dynamic covalent cross-links, previously thermoplastic materials exhibit robust mechanical properties characteristic of conventional thermosets yet maintain their reprocessability at high temperatures. Using reactive batch processing, we upcycled virgin and waste low-density and high-density polyethylene into covalent adaptable networks (CANs) via melt-state, free-radical grafting of a cross-linker capable of dynamic dialkylamino disulfide (BiTEMPS) chemistry onto polymer chains. Unlike PE thermosets, our PE CANs are reprocessable and recover their thermomechanical properties after reprocessing. We have further shown that, in the absence of crystallinity, high-temperature creep behavior of the CANs is dominated by the exclusively dissociative reversible dynamic chemistry of the cross-linker. This observation also demonstrates the utility of this dissociative dynamic chemistry of high activation energy at suppressing creep in networks exhibiting different viscoelastic behavior. We will also describe cases of other thermoplastics that are able to be upcycled into CANs using our simple method.

4:20 PM

Rheology and Spinnability of Polyvinylpyrrolidone Solutions

Louis Edano (University of Illinois Chicago)

We examine spinnability and centrifugally-spun fiber properties for polyvinylpyrrolidone (PVP) by first focusing on the influence of molecular weight and dispersity, and the choice of solvent. A small fraction of high molecular weight (UHMW) PVP is incorporated to illustrate extensibility-enriched spinnability and highlight how nearly similar shear, but quantitatively stronger and different extensional rheology response changes the spinnability outcomes. To elucidate the influence of solvent properties, we vary ethanol content in spinning dope comprising aqueous PVP solutions. We rely on a bespoke centrifugal force spinning (CFS) set-up that allows spinning from two symmetrically placed nozzles onto a collector using matched processing parameters, but variable polymer-solvent concentrations.

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High School Outreach Program

This special high school program is being run in parallel with the American Institute of Chemical Engineers (AIChE) 15th Annual Midwest Regional Conference. AIChE and UIC would like to expose students to the profession of chemical engineering and engineering in general and give them the opportunity to interact with professional engineers, engineering students, and faculty. We hope you come away from this program with some idea of what engineers do, how they touch your life, and whether you would like to pursue an engineering career.

8:45-9:45 **Engineering Expo** (SCE Tower 3rd Floor Hallway, 302)
- Meet with current engineering students and see some of their projects

9:45-10:00 **Introduction** (SCE Tower 302)
- Overview of the schedule for the day

10:00-11:30 Groups will split into two groups and rotate through the following 40 minute activities

Presentation on Engineering Careers (SCE Tower 605)
- Learn about how engineers contribute to all aspects of society

Team Building Exercise (SCE Tower 603/613)
- Work with other students to complete a hands-on engineering-related task

11:30-12:00 **Engineering Lunch** (SCE Illinois A & Illinois B)
- Opportunity for one-on-one discussions with engineering professionals and students.

12:15-12:45 **Keynote Speaker** (SCE Tower 302)
- Valarie King-Bailey, MBA – CEO of OnShore Technology Group

12:45-1:30 **Engineering Panel Session** (SCE Tower 302)
- Learn about the day-to-day activities of practicing engineers and engineering students. Time to ask your most burning questions.

Valarie King-Bailey, MBA

Valarie King-Bailey, MBA is the CEO of OnShore Technology Group, an independent Chicago-based software and professional services consultancy specializing in the development and delivery of software and professional services targeted towards the life sciences industry. OnShore's software platform, ValidationMaster™ is used by leading companies across the globe to test enterprise software applications in compliance with global regulatory requirements. OnShore has been listed twice, in 2021 and 2022 on the prestigious INC 5000 list of the fastest growing companies in America and received the INC Top Female 100 founders award. In 2022, Valarie received the Chancellors Entrepreneurial Achievement Award from the University of Wisconsin – Madison. Valarie has worked for leading global companies such as QUMAS Limited (Ireland), EMC/Documentum, Abbott Laboratories, and U.S. Steel; South Works. At QUMAS, an Irish-based software company, she served as Chief Marketing Officer where she was responsible for all global tactical and strategic marketing initiatives in addition to the development of their validation toolkit. Valarie founded OnShore Technology Group in 2004. Valarie is a fierce STEM advocate and speaks to young people at venues throughout the U.S. Ms. King- Bailey holds an M.B.A. in Information Systems from Keller Graduate School of Management (1985) and a B.S. in Civil and Environmental Engineering from the University of Wisconsin Madison (1982). She is a member of the American Society of Civil Engineers, Society of Women Engineers (SWE), National Society of Black Engineers, National Girls Collaborative Project for STEM education, Regulatory Affairs Professional Society (RAPS), and a U.W. College of Engineering Advisory Board Member. Valarie also server as the program director of the DePaul University Women's entrepreneurs institute in Chicago.

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AIChE MIDWEST REGIONAL CONFERENCE

MRC 2024

16th Annual AIChE Midwest Regional Conference

Chicago - Spring 2024

For programming and volunteer opportunities for next year's conference, please contact the AIChE Chicago Section at aichechicago@gmail.com

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Young Professionals Social

Come and join your fellow YP's in celebrating a successful conference by relaxing at the YP Social for networking, drinks, and great conversation! Feel free to join us even if you weren't able to make it to the conference!

What: YP Social after the 15th Annual Midwest Regional Conference @ UIC
When: Wednesday, April 12th, 5:30PM – 8:30PM
Where: Bar Louis
1325 S Halsted St. Chicago, IL
Contact: Ruben @ 312-351-2496

Hosted by AIChE Chicago Young Professionals Committee (YPC)

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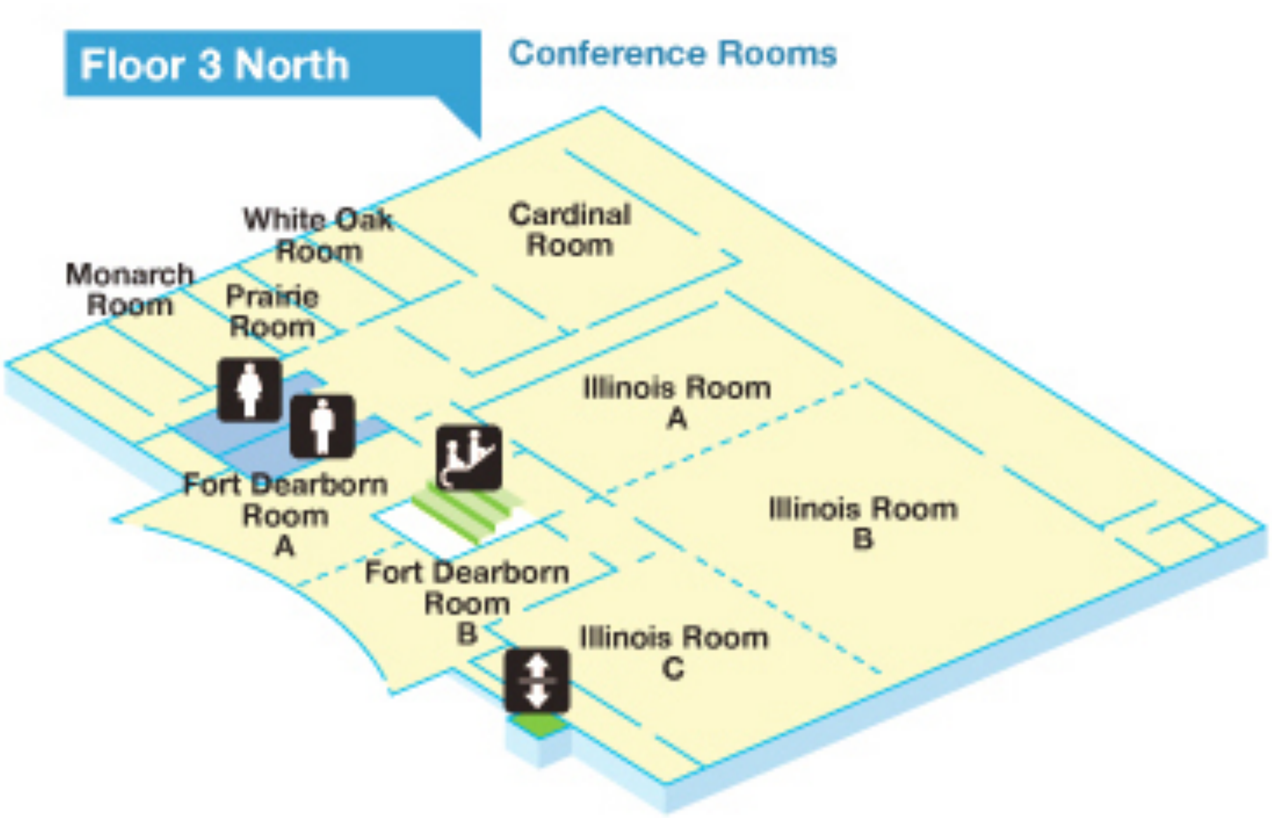
Conference Map



Room	Description
Cardinal Room	Keynote Talks (Day 1 and 2) Dinner (Day 1) Lunch (Day 2)
White Oak Room	Technical Sessions: Track 1 (Day 1 & 2)
Illinois C	Technical Sessions: Track 2 (Day 1 & 2)
Illinois Room AB	Lunch (Day 1)
Illinois Room A	Poster Session (Day 1)
Fort Dearborn Room AB	Registration Sponsor Exhibits Coffee/Breakfast/Networking Breaks
Prairie Room	Conference Organizer Room