16th Annual
AIChE Midwest Regional Conference

March 5-6, 2024

https://www.aiche.org/conferences/midwest-regional-conference/2024

Organized by the AIChE Chicago Local Section, AIChE Global and the Illinois Institute of Technology

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Conference Overview

The AIChE Midwest Regional Conference (MRC) continues into its 16th year. Organized by the **AIChE Chicago Local Section, AIChE Global** and the **Illinois Institute of Technology**, 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:

5 Keynote Lectures:

- **Mike Pires,** *Vice President, North and Central Commercial Enablement, Americas Air Products*
- ***Venkat Srinivasan,*** *Director of the Argonne Collaborative Center for Energy Storage Science, Argonne National Laboratory*
- **Karen Vilas,** *President, FORTRESS Protective Buildings*
- **Jeff Greenley,** *Professor of Chemical Engineering, Purdue University*
- **Meenesh Singh,** *Professor of Chemical Engineering, University of Illinois at Chicago*

The conference contains **14 technical sessions** featuring over **46 oral presentations.** The Tuesday evening program is combined with the ***AIChE Chicago Local Section Monthly 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 **Marty Gonzalez** (Innovation and Technology Principal at BP) as keynote speaker and includes lunch where students can interact with practicing engineers.

On behalf of the conference planning committee, we welcome you to the 16th Annual AIChE Midwest Regional Conference and hope you will take advantage of all the opportunities it has to offer.

Belma Demirel
Conference Chair
bp

Hadjira Iddir
Conference Co-Chair
Honeywell UOP

Jason Wu
Programming Chair
Honeywell UOP

Hakim Iddir
Programming Co-Chair
Argonne National Laboratory

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Program at a Glance (Day 1)

Tuesday, March 5, 2024

8:15 – 8:30 AM **Conference Introduction** (Ballroom)

8:30 – 9:30 AM **1st Morning Keynote** (Ballroom)
Mike Pires*, Air Products*

9:30 – 9:50 AM **Break**

9:50 – 11:30 AM **Session I**

Track 1	**Track 2**
Energy Storage I (Alumni Lounge)	Green Engineering (Hermann Lounge)

11:30 AM– 12:45 PM **Lunch with High School Outreach** (Ballroom & Expo Room)

12:45 – 1:45 PM **2nd Keynote** (Ballroom)
Venkat Srinivasan*, Argonne National Laboratory*

1:45 – 2:00 PM **Break**

2:00 – 3:15 PM **Session II**

Track 1	**Track 2**
Energy Storage II (Alumni Lounge)	Process Safety I (Hermann Lounge)

3:15 – 3:30 PM **Break**

3:30 – 4:20 PM **Session III**

Track 1	**Track 2**
Fluid Properties, Fluid Dynamics & Transport Phenomena (Alumni Lounge)	Process Safety II (Hermann Lounge)

4:20 – 5:45 PM **Poster Session** (Gallery Lounge)

5:45 – 7:30 PM **Chicago Section Dinner** (Ballroom)
Dinner Keynote – Karen Vilas, *BakerRisk*

Program at a Glance (Day 2)

Wednesday, March 6, 2024

8:25 – 8:30 AM **Conference Introduction** (Ballroom)

8:30 – 9:30 AM **1st Morning Keynote** (Ballroom)
Jeff Greeley*, Purdue University*

9:30 – 9:50 AM **Break**

9:30 – 11:30 AM **Session I**

Track 1	**Track 2**
Advances in Refining / Materials (Alumni Lounge)	Bioengineering and Nanotechnologies (Hermann Lounge)

11:30 AM– 12:45 PM **Lunch (Ballroom)**

12:45 – 1:45 PM **Afternoon Keynote** (Ballroom)
Meenesh Singh**,** *UIC*

1:45 – 2:00 PM **Break**

2:00 – 3:15 PM **Session II**

Track 1	**Track 2**
Machine Learning / Optimization I (Alumni Lounge))	Catalysis I (Hermann Lounge)

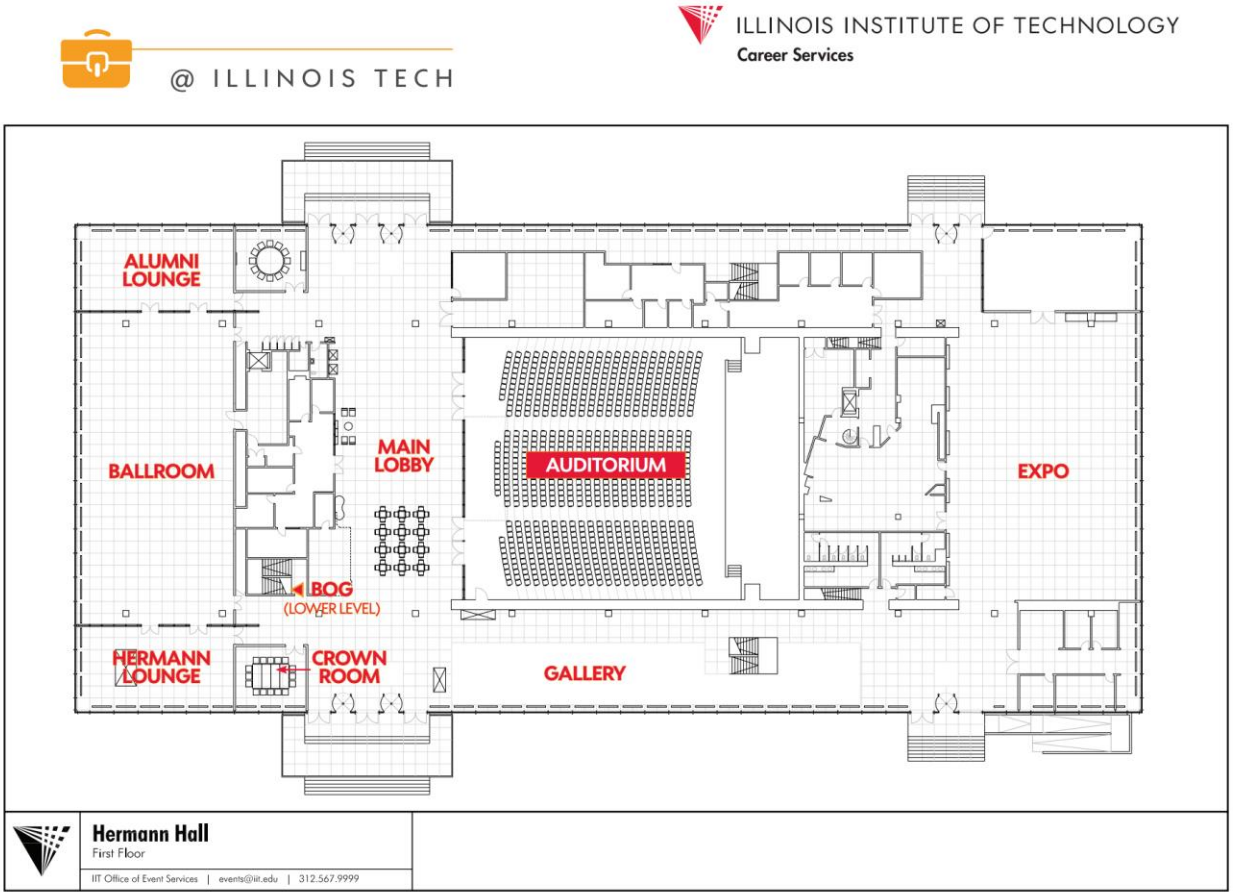
3:15 – 3:30 PM **Break**

3:30 – 4:45 PM **Session III**

Machine Learning / Optimization II (Alumni Lounge))	Catalysis II (Hermann Lounge)

4:45 – 6:00 PM **Happy Hour Hosted by CLS YP** (Cork and Kerry at the Park, *offsite*)

Conference Map



Keynote Speakers

Tuesday Morning Keynote: 8:30 AM, March 5, 2024

The Future is now… Hydrogen's role in the Energy Transition

Mike Pires, *Vice President, North and Central Commercial Enablement, Americas Air Products*

Mike Pires is responsible for the growth and profitability of the company's Industrial Gases business in the Northern U.S. In addition, he has executive leadership responsibility for the Americas Strategy, Marketing and Technology, and Americas Procurement and Strategic Sourcing organizations.

Mr. Pires has over 25 years of experience in the industrial gas industry, working for BOC Gases, ABCO Welding & Industrial Supply, Gerdau, and Air Products. He began his career at Air Products as a senior account executive. From 2013-2017, Mr. Pires served as Midwest area manager and was pivotal in improving the company's strategically acquired carbon dioxide business and driving meaningful growth in the existing Industrial Gases business. He was named Commercial Director, Northern Region, in 2017, followed by Director, Americas Strategy, Marketing and Technology, in 2019. In 2020, Mr. Pires was appointed Vice President and General Manager, North Region, Americas before assuming his current position.

Mr. Pires holds a B.S. degree in business from Muhlenberg College and an MBA from Lehigh University.

Tuesday Afternoon Keynote: 12:45 PM, March 5, 2024

Status of Batteries for Transportation and Grid Decarbonization

Venkat Srinivasan, *Director of the Argonne Collaborative Center for Energy Storage Science, Argonne National Laboratory*

Venkat Srinivasan is the Director of the Argonne Collaborative Center for Energy Storage Science (ACCESS) and Deputy Director of the Joint Center for Energy Storage Research (JCESR).
ACCESS provides the vision and coordinates the energy storage programs at Argonne and serves as a point of entry for industry to take advantage of the unique capabilities and facilities at Argonne to solve their problems in energy storage. JCESR is a national program led by Argonne that focuses on next-generation energy storage research that goes beyond lithium-ion technology.

He is a former staff scientist at Lawrence Berkeley National Laboratory. His research interest is developing next-generation batteries for vehicle and grid applications, among other things. Dr. Srinivasan and his research group develop continuum-based models for battery materials and combine them with experimental characterization to help design new materials, electrodes, and devices.

In addition to his research, Dr. Srinivasan is interested in moving technologies to market and has been exploring ways to develop an ecosystem, focused on batteries, to accelerate technology commercialization. In this role, Dr. Srinivasan conceived the idea of CalCharge, a one-of-a-kind public-private partnership in energy storage.

Dr. Srinivasan has previously served as the technical manager of the Batteries for Advanced Transportation Technologies (BATT) Program, as the acting director of the BATT program, as department head of the Energy Storage and Distributed Resources (ESDR) department at LBNL, and the interim director of the ESDR Division at LBNL. Dr. Srinivasan joined the scientific staff at LBNL in 2003 after postdoctoral studies at the University of California, Berkeley and Pennsylvania State University. He received his PhD from the University of South Carolina in 2000.

He is also the author of a popular battery blog titled, “This Week in Batteries.”

Tuesday Evening Keynote: 6:30 PM, March 5, 2024

Leadership, Innovation, and the Pursuit of Legacy. From Chemical Engineer to FORTRESS Protective Buildings

Karen Vilas, *President, FORTRESS Protective Buildings*

Recognized globally as a leader in process safety, Karen's career has focused on Facility Siting Studies and Quantitative Risk Analyses for oil & gas and petrochemical facilities. Beginning in 2019, Karen helped to establish the Low Carbon Energy service offerings within BakerRisk, leading the Hydrogen and Hydrogen Carriers initiatives within the organization. Karen has been an active member of AIChE and AIChE's Center for Hydrogen Safety for many years including working with the CHS Organizing Committee in 2022.

In August 2022, Karen became President of FORTRESS Protective Buildings, a wholly owned subsidiary of BakerRisk. As a new market offering, FORTRESS provides multi-hazard resistant buildings (MRBs) for facilities handling hazardous materials. Since joining FORTRESS, Karen has leveraged her background and collaborated with clients to provide risk mitigation and risk management solutions by focusing on providing high quality, highly protective buildings to industries that handle flammable, toxic, or explosive materials.

<u>Wednesday Morning Keynote</u>: 8:30 AM, March 6, 2024

First principles treatments of heterogeneous electrocatalysis – reactivity trends and electrocatalyst structure

Professor Jeff Greenley, *Charles Davidson Professor of Chemical Engineering at Purdue University*

Prof. Jeffrey Greeley obtained his PhD from Department of Chemical Engineering at the University of Wisconsin-Madison in 2004. Following two years of postdoctoral work at the Technical University of Denmark, he moved to Argonne National Laboratory, where he served for six years as a staff scientist in the Center for Nanoscale Materials before joining the Davidson School of Chemical Engineering at Purdue University in 2013.

Professor Greeley's research group at Purdue focuses on the use of first principles Density Functional Theory calculations to understand chemical processes at surfaces and interfaces. His primary interests are in the areas of heterogeneous catalysis and electrocatalysis, and his work has led to the prediction and successful testing of improved heterogeneous catalysts and electrocatalysts for reactions of interest in fuel cells, electrolyzers, and related devices. He has published over 200 research articles in this field.

Wednesday Afternoon Keynote: 12:45 PM, March 6, 2024

Nitrogen Electrochemistry to Support DOE's Energy Earthshots

Meenesh Singh, *Professor, Department of Chemical Engineering, University of Illinois at Chicago*

Dr. Singh is an associate professor in the Department of Chemical Engineering and the director of the Materials and Systems Engineering Lab (MaSEL) at the University of Illinois Chicago (UIC), where his research group is developing state-of-the-art computational and experimental tools to solve grand challenges of the 21st century: (1) develop carbon sequestration methods, (2) manage the nitrogen cycle, (3) provide access to clean water, and (4) engineer better medicines.

Dr. Singh obtained his B. E. degree in chemical engineering from Sardar Patel University in 2005, M. Tech. Degree in chemical engineering from Indian Institute of Technology Bombay in 2008 and Ph.D. in chemical engineering from Purdue University in 2013. His research resulted in 7 patents (3 licensed), > 60 publications, 2 book chapters, 5 open-source software, >100 presentations at international conferences, and 28 invited talks. His research lab has been awarded multi-million dollars to support the development of disruptive technologies through a strong/continued collaboration with 7+ multinational companies. He has supervised 5 Ph.D. students and is currently advising 5 Ph.D. students, 3 postdocs, and several undergraduate students. He is a faculty advisor for AIChE Chem-E-Car and an editorial board member for 5 scientific journals, including Chemical Engineering Research & Design (Elsevier) and Sustainable Chemistry (MDPI). He is also the CTO of eN-RAMPS, a company that focuses on the scale-up and commercialization of technologies developed in his lab at UIC.

Session Presentations (Day 1)

Tuesday, March 5, 2024

Conference Welcome

8:15 AM AIChE Chicago Introduction

McKay Rytting (Local Section Chair, EY-Parthenon)

8:25 AM Conference Introduction

Belma Demirel (Conference Chair, bp)
Hadjira Iddir (Conference Co-Chair, Honeywell UOP)

Morning Keynote

8:30 AM Keynote Introduction

Jason Wu (Programming Chair, Honeywell UOP)

8:35 AM

The Future is now… Hydrogen's role in the Energy Transition
Mike Pires (Air Products)

Track 1 - Energy Storage I

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

9:50 AM

Enhancing Solid Polymer Electrolytes for All-Solid State Batteries
Ahmad Helaley *and Xinhua Liang* (Washington University in St. Louis)

10:15 AM

Predicting Energy Consumption in Lithium-Ion Gigafactories
Kevin Knehr[1]*, Joseph Kubal*[1]*, SeungRyeol Yoon*[2]*, HyeongRyul Jeon*[2]*, Whan Jin Roh*[2] *and Shabbir Ahmed*[1] ([1]Argonne National Laboratory, [2]Top Material Co., Ltd.)

10:40 AM

Enhanced Performance of Lithium-Ion Batteries By Atomic Layer Deposition
Xinhua Liang (Washington University in St. Louis**)**

11:05 AM

Earth Abundant Elements Distribution and Domain Structure in Li-Rich Mn-Rich Based Cathode Materials
Juan Garcia *and Hakim Iddir* (Argonne National Laboratory**)**

Track 2 - Green Engineering

Chair: *Trevor Lardinois* (Exponent)

9:50 AM

Validation of Passive Solar Dehydrator for Fruit Drying Applications: A Pineapple Study
Katherine Kuhn*, Paige Bowman, Charles Strnad* **(**Milwaukee School of Engineering**)**

10:15 AM

Numerical Modeling of Electrochemical CO_2 Reduction Reaction (eCO_2RR) in a Batch-Cell
Ahmad Ijaz (Illinois Institute of Technology**)**

10:40 AM

Breaking Frontiers in Selective Electroreduction of CO2 to Ethylene Under Controlled Catalyst Regeneration
Nitin Minocha, PhD *and Meenesh R. Singh* **(**University of Illinois, Chicago**)**

11:05 AM

Electrochemical One-Pot Systems for Advancing Carbon Capture and Utilization in Simulated Flue Gas Conditions
Rohan Sartape*, Vamsi V. Gande and Meenesh R. Singh* (University of Illinois, Chicago)

Afternoon Keynote

12:45 PM Keynote Introduction
Hakim Iddir (Programming Co-Chair, Argonne National Laboratory)

12:50 PM
Status of Batteries for Transportation and Grid Decarbonization
Venkat Srinivasan (Argonne National Laboratory)

Track 1 - Energy Storage II

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

2:00 PM
Assessing Particle Degradation in Thermochemical Energy Storage through Imaging
Spenser Vasich (Michigan State University)

2:25 PM
Upgrading Sustainable Materials into Specialized Flow Battery Chemistries
Patrick Sullivan (Flux XII Inc.)

2:50 PM
Negative Electrodes Performance of Lead-Acid Batteries: Analysis from Modeling Cyclic Voltammetry Responses
Mohammed Effat, *Kevin Knehr*,*Crystal Ferels*, *Chaudhari Nikhil, Pietro Lopes* and *Tim Fister*
(Argonne National Laboratory)

Track 2 – Process Safety I

Chair: *Jessica Morris* (BakerRisk)
Co-Chair: *Zac Adesanya* (UIC)

2:00 PM
Important Characteristics of an Effective Process Safety Knowledge Management System
Tekin Kunt *and Anthony Do* (PSRG Inc.)

2:25 PM
Process Safety of Combustible Dust, the Dust Hazard Analysis
Danielle Kittaka *and Timothy Cullina*
(Risk Management, Fauske and Associates)

2:50 PM
Hazardous Waste Generators and Treatment Facilities: Hazardous Waste Characteristics, Rcra, and Treatment Technologies
Trevor Lardinois and *Brenton Cox*
(Exponent, Inc.)

Track 1 - Fluid Properties, Fluid Dynamics & Transport Phenomena

Chair: *Hadjira Iddir* (Honeywell UOP)
Co-Chair: *Paul Vesely* (Spraying Systems Co.)

3:30 PM
Prediction of Densities in Fluidized Bed Strippers for Various Types of Internals
Allan Issangya *and* Surya Karri
(Particulate Solid Research, Inc.)

3:55 PM
Using Network Theory to Gain Novel Insights on Flow and Dynamics of Dense Suspensions: Node and Edge Centric Methods
Alessandro d'Amico*, Sidong Tu and Abhinendra Singh* (Case Western Reserve University**)**

Track 2 – Process Safety II

Chair: *Jessica Morris* (BakerRisk)
Co-Chair: *Zac Adesanya* (University of Illinois, Chicago)

3:30 PM
Hazardous Area Classification Best Practices
Calvin Doty (BakerRisk**)**

3:55 PM
Shelter-in-Place Guidance/Best Practices to Tackle Toxic Exposure
Sajjid Odeh (BakerRisk)

Poster Session

Chair: *Adam Kanyuh* (Poster Session Chair)

4:20 PM

Characterizing and Engineering Homologs of a Template-Independent DNA Polymerase for Signal Recording Applications
Teresa Rojas Rodríguez*, Marija Milisavljevic and Keith Tyo,* (Northwestern University)

Quantum Mechanical Modeling of Enzyme Promiscuity: Application to Carboligases
Geoffrey Bonnanzio (Northwestern University)

Process Design, Scaling, and Integration of Catalytic Reactor and Separation Sections for Dehydration of Lactic Acid to Acrylic Acid
Christopher P. Nicholas, *Zac Pursell* (Låkril Technologies Corporation)

Chicago Section Monthly Technical Dinner and Dinner Keynote

5:45 PM
Dinner

6:15 PM
Section Announcements
McKay Rytting (Local Section Chair, EY-Parthenon)

Dinner Keynote

6:25 PM Keynote Introduction
Jessica Morris (Facilities and Logistics Chair, BakerRisk)

6:30 PM

Leadership, Innovation, and the Pursuit of Legacy. From Chemical Engineer to FORTRESS Protective Buildings
***Karen Vilas* (**President, FORTRESS Protective Buildings)

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Session Presentations (Day 2)

Wednesday, March 6, 2024

Conference Welcome

8:25 AM Conference Introduction
Belma Demirel (Conference Chair, bp)
Hadjira Iddir (Conference Co-Chair, Honeywell UOP)

Morning Keynote

8:30 AM Keynote Introduction
Hakim Iddir (Programming Co-Chair, Argonne National Laboratory)

8:35 AM
First principles treatments of heterogeneous electrocatalysis – reactivity trends and electrocatalyst structure
Jeff Greeley (Purdue University)

Track 1 – Advances in Refining / Materials

Chair: *Jason Wu* (Honeywell UOP)
Co-Chair: *Nick Shulman* (Exponent, Inc.)

9:50 AM
Integration of reconciliation infrastructure for refinery scheduling model tuning
Sean R. Werner, PhD (ExxonMobil Technology and Engineering Company)

10:20 AM
Metal-Organic Frameworks at Numat™: A Decade of Innovation, High-Tech Manufacturing, and Future Growth.
William Morris (NuMat)

10:50 AM
Petrochemical Transformation: Overcoming Challenges in the Olefins Industry with Naphtha to Ethane/Propane (NEP) Technology
Robert Szczesniak*, Greg Funk* (Honeywell UOP)

Track 2 – Bioengineering and Nanotechnologies

Chair: *Meltem Demirtas* (Argonne National Laboratory)
Co-Chair: *Wujie Zhang* (Milwaukee School of Engineering)

9:50 AM
Long-Term Antibody Release Polycaprolactone Capsule and the Release Kinetics in Natural and Accelerated Degradation
TJ Waterkotte*, Xingyu He, Apipa Wanasthop, S. Kevin Li and Yoonjee Park* (University of Cincinnati)

10:20 AM
High-Throughput Screening of *E. coli* Ghosts Against 314 G-Protein Coupled Receptors (GPCRs)
Christopher Vidmar *and Jennifer Fiegel* (University of Iowa)

10:50 AM
A Wide Look at MXene-based CO2 Reduction Electrocatalysts: Pioneering Pathways for Green Formaldehyde Production
Sixbert P. Muhoza[1] *Shiba P. Adhikari*[1] *Francisco Lagunas Vargas*[1]*, Anupma Thakur*[2]*, Songge Yang*[3]*, Yu Zhong*[3]*, Babak Anasori*[2] *and Zachary D. Hood*[1] ([1]Argonne National Laboratory, [2]Purdue University, [3]Worcester Polytechnic Institute)

Afternoon Keynote

12:45 PM Keynote Introduction

Jason Wu (Programming Chair, Honeywell UOP)

12:50 PM

Nitrogen Electrochemistry to Support DOE's Energy Earthshots

Meenesh Singh (Professor, Department of Chemical Engineering, University of Illinois at Chicago)

Track 1 – Machine Learning / Optimization I

Chair: *Mohammed Effat* (Argonne National Laboratory)
Co-Chair: *David Neira* (Purdue University)

2:00 PM

Early Detection of Catalyst Transfer Pipe Plugging Using Temperature Signal Analysis

Holly Butcher*, Mahesh Kumar Gellbaoina, and* ***Louis Lattanzio*** (Honeywell UOP)

2:25 PM

Importance Learning Analysis of Ethylene Polymerization By a Single-Atom Cr/SiO_2Catalyst

Changhae Andrew Kim*, Armin Shayesteh Zadeh and Baron Peters* (University of Illinois Urbana-Champaign)

2:50 PM

Logic-Based Discrete-Steepest Descent: A Solution Method for Process Synthesis Generalized Disjunctive Programs

Albert Lee**[1]***, Daniel Ovalle[2], David Alejandro Linan Romero[3] Luis Ricardez-Sandoval[3], Jorge M. Gomez[4], Ignacio Grossmann[2] and David E. Bernal Neira[5]*
([1]Purdue University, [2]Carnegie Mellon University, [3]University of Waterloo, [4]Universidad de los Andes, [5]NASA Ames Research Center)

Track 2 – Catalysis I

Chair: *Aditya Prajapati* (Lawrence Livermore National Lab)
Co-Chair: *Shri Dawande (Motorola Solutions*)

2:00 PM

Highly Selective and Stable Pt-Co Bimetallic Catalysts Prepared By Atomic Layer Deposition for Unsaturated Aldehyde Hydrogenation

Kaiying Wang*[1], Xiaofeng Wang[2] and Xinhua Liang[1]* ([1]Washington University in St. Louis, [2]Missouri University of Science and Technology)

2:25 PM

Two-Phase Reactors and Population Balance Models for Polymer Upcycling

Changhae Andrew Kim*[1], Chinmay A. Sahasrabudhe[1], Yi-Yu Wang[2], Ryan Yappert[1], Andreas Heyden[3], Wenyu Huang[2,4], Aaron Sadow[2,4] and Baron Peters[1]* ([1]University of Illinois Urbana-Champaign, [2]Iowa State University, [3]University of South Carolina, [4]U.S. DOE Ames Laboratory)

2:50 PM

Process Design, Scaling, and Integration of Catalytic Reactor and Separation Sections for Dehydration of Lactic Acid to Acrylic Acid

Christopher P. Nicholas *and Zac Pursell*
(Lakril Technologies Corporation)

Track 1 – Machine Learning / Optimization II

Chair: *Mohammed Effat* (Argonne National Laboratory)
Co-Chair: *David Neira* (Purdue University)

3:30 PM

Optimizing Reverse Electrodialysis Process for Renewable Electricity Generation from Salinity Gradient

Carolina Tristan*[1], Marcos Fallanza[2], Raquel Ibañez[2] and David E. Bernal Neira[1,3,4]*
([1]Purdue University, [2]University of Cantabria, [3]NASA Ames Research Center, [4] Universities Space Research Association – Research Institute of Advanced Computer Science)

3:55 PM

Graph-Based Representations and Applications to Process Simulation

***Yoel Cortes-Pena*[1]** *and and Victor M. Zavala*[2]
([1]DOE, University of Illinois at Urbana-Champaign, [2]University of Wisconsin-Madison)

4:20 PM

A Water-Energy-Food Nexus Framework to Improve Resource Security

Brenda Cansino Loeza[1], Aurora Del Carmen Munguia Lopez[1], Jose Ponce-Ortega[2] and Victor M. Zavala[1] ([1]University of Wisconsin-Madison, [2]Universidad Michoacana de San Nicolas de Hidalgo)

Track 2 – Catalysis II

Chair: *Aditya Prajapati* (Lawrence Livermore National Lab)
Co-Chair: *Shri Dawande* (Motorola Solutions)

3:30 PM

DFT Analysis of Surface-Bound Nitrogen Species Under N_2 Plasma Exposure

Chang Yan*, Garam Lee, David Go, Casey O'Brien and William Schneider*
(University of Notre Dame)

3:55 PM

Structure and Tunable Nature of Heterogenized Molecular Catalysts Developed By Oxidative Grafting

Jacklyn Hall*, Alon Chapovetsky, Uddhav Kanbur, A. Jeremy Kropf, Massimiliano Delferro and David Kaphan*
(Argonne National Laboratory)

Presentation Abstracts (Day 1)

Tuesday, March 5, 2024

Tuesday Morning Keynote Session

8:30 AM

The Future is now… Hydrogen's role in the Energy Transition

Mike Pires (Vice President, North and Central Commercial Enablement, Americas Air Products)

Extreme temperatures, droughts, and an increased frequency of powerful storms. All are signs of the impact of climate change. To stave off a continued worsening of climate issues, more must be done, and done quickly to decarbonize and reduce overall CO2 emissions. The good news. The tools needed to bring about significant change are available today. The promise of renewable energy and electrification is real, but that alone cannot accommodate all the needs of daily living in the 21st century while growing our economy and achieving our climate goals. That's where hydrogen comes in. Hydrogen is the best solution to decarbonize hard-to-abate sectors, such as heavy-duty transportation, or steel making or the production of chemicals. In this session, I will share the powerful impact hydrogen will have on the ongoing energy transition. I will share information about real projects, in progress today, that will help us achieve our goals and generate a cleaner future. I will also discuss the opportunities that exist for the current and future generation of engineers and their part in solving the challenge of climate change.

Track 1

Energy Storage I

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

9:50 AM

Enhancing Solid Polymer Electrolytes for All-Solid-State Batteries

Ahmad Helaley, Xinhua Liang (Department of Energy, Environmental & Chemical Engineering, Washington University in St. Louis, MO)

Solid polymer electrolytes (SPEs) have emerged as pivotal components in the development of all-solid-state batteries, offering enhanced safety and design flexibility. In this study, we focus on optimizing the electrochemical performance of SPEs through the incorporation of poly(ethylene oxide) (PEO) blended with amorphous poly(propylene glycol) (PPG) and poly(ethylene glycol-ran-propylene glycol) (PEG-PPG). The addition of PEG/PPG to PEO has been found to reduce crystallinity, facilitating improved lithium ion diffusion within the SPE. This not only broadens the temperature range for optimal battery operation but also reduces the electrolyte/electrode interfacial resistance, thereby enhancing electrochemical stability. Comparative studies revealed that SPEs based on PEO blended with 7% PEG-PPG or PPG exhibited excellent charge/discharge cycling stability. At a current rate of 0.2 C, these systems demonstrated maximal discharge capacities of 165 mAh g^{-1} and 162 mAh g^{-1} at 60 °C and 125 °C, respectively. The PEG-PPG-based SPE outperformed its PPG counterpart, showcasing superior electrochemical performance and a broader temperature range attributed to its longer polymer chain. However, concentrations exceeding 7 wt.% PEG-PPG/PPG resulted in decreased crystallinity and compromised electrochemical performance. This nuanced balance between polymer components offers improved ionic conductivity, interface stability, and electrolyte compatibility with electrodes, presenting a highly suitable solution for high-demand applications in lithium-ion batteries. This study contributes valuable insights into tailoring SPEs for enhanced battery performance.

10:15 AM

Predicting Energy Consumption in Lithium-Ion Gigafactories

Kevin Knehr[1], Joseph Kubal[1], SeungRyeol Yoon[2], HyeongRyul Jeon[2], Whan Jin Roh[2] and Shabbir Ahmed[1], ([1]Argonne National Laboratory, Lemont, IL, [2]Top Material Co., Ltd., Republic of South Korea)

The energy consumption of a lithium-ion battery gigafactory, in $Wh_{consumed}/Wh_{cell}$, is an important value used in life cycle analyses of electric vehicles. The energy consumption also has important ramifications on construction, as it impacts the cost and infrastructure requirements of the plant. This presentation will discuss recent work focused on predicting the energy consumption of lithium-ion gigafactories. The results from three case studies of plants manufacturing $LiNi_{0.83}Co_{0.11}Mn_{0.06}O_2$-Graphite (NCM83-G) cells at rates of 5, 25, and 50 GWh/yr are used to investigate the main drivers of energy consumption in a plant. Data from the studies are used to generate scaling factors and baseline energy consumption values for each step in the manufacturing process. These values are input into the Battery Performance and Cost Model (BatPaC), a freely available tool for battery sizing and cost estimations, to study the manufacturing processes, material properties, and cell design decisions which most influence energy consumption. The presentation will also discuss the development of an analytical expression that can be used for first-pass estimation of the energy consumption in a lithium-ion battery gigafactory. The expression depends on the properties and manufacturing rates of the cell, making it a useful tool for early-stage engineering estimates.

10:40 AM

Enhanced Performance of Lithium-Ion Batteries By Atomic Layer Deposition

Xinhua Liang (Department of Energy, Environmental & Chemical Engineering, Washington University in St. Louis, St. Louis, MO)

Surface modification has been widely considered as an effective strategy to boost cycle-life and enhance conductivity of electrode particles for lithium-ion batteries (LIBs). Atomic layer deposition (ALD) is a layer-by-layer thin film coating technique. Through ALD, a conformal ultrathin coating with controllable thickness can provide initial protection for surface of active materials. We use scalable fluidized bed reactor to realize conformal thin film coating on primary particles. In this presentation, I will discuss our recent results of performance enhancement of lithium-ion batteries by ALD, including conductive thin film coating on electrode particles, simultaneous doping and thin film coating on electrode particles, and recovery of degraded Ni-rich NMC811 particles by ALD.

11:05 AM

Earth Abundant Elements Distribution and Domain Structure in Li-Rich Mn-Rich Based Cathode Materials

Juan Garcia, Hakim Iddir (Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL)

The nature and morphology of domains in composite Li-rich Mn-rich (LMR) cathode materials play a major role in their electrochemical performance and degradation. This work presents a theoretical study on the influence of earth abundant (EA) dopant on the domain structure of cathode materials. From density functional theory, machine learned potentials and thermodynamic analysis, we found that the configuration with the highest probability of occurrence at room temperature is a composite of L_2MnO_3-like and $LiNi_{0.5}Mn_{0.5}O_2$ zigzag domains. At higher temperatures, however, a mix of composite and “disordered” configurations are also possible. Site preference of EA dopants and their effect on the activation process in LMR materials will be discussed.

Track 2
Green Engineering

Chair: Trevor Lardinois (Exponent)

9:50 AM

Validation of Passive Solar Dehydrator for Fruit Drying Applications: A Pineapple Study

Katherine Kuhn, Paige Bowman, Charles Strnad (Milwaukee School of Engineering)

A major struggle in the Sub-Saharan African region is food preservation and storage. To alleviate this issue, the use of solar dehydration trays has been proposed.

These trays are advantageous in the Sub-Saharan African region because they are cheap, require no electricity, and utilize the abundant natural resource of solar heat. This study seeks to further validate the quality of fruit samples produced by passive dehydration. Solar-dehydrated samples were compared to freeze-dried samples, as they represent the gold standard of fruit preservation. To mimic the Saharan African environment (temperature and humidity) a psychrometric chamber was utilized. In this environment, samples of pineapple were dehydrated and subjected to testing against fresh and freeze-dried samples. The average water content for solar-dehydrated pineapple was found to be 10%, which is below the standard threshold of 20%. Vitamin C content, iron content, and dissolved solids were found to be comparable between fresh and freeze-dried samples. Moreover, microbial testing indicated that there was no introduction of microbial contamination during the solar dehydration process. Sensory evaluation (colorimetry) indicated solar-dehydrated samples were even superior to freeze-dried samples. In summary, solar dehydration is a viable method of fruit preservation.

10:15 AM

Numerical Modeling of Electrochemical CO_2 Reduction Reaction (eCO_2RR) in a Batch-Cell

Ahmad Ijaz (Department of Chemical & Biological Engineering, Illinois Institute of Technology, Chicago, IL)

Among various technologies to utilize captured CO_2, electrochemical conversion of CO_2 into value added products is emerging as a potential technology. Batch-cell (batch-electrolyzer) is used to study the electrochemical CO_2 reduction reaction (eCO_2RR) and to quickly assess an electrochemical catalyst. Therefore, a multiphysics numerical model is developed for batch-cell with glassy carbon electrode (GCE) to gain fundamental understanding of its operation that could help to optimize its performance. Electrochemical parameters are obtained from the experimental findings of catalyst $CuAg_{0.5}Ce_{0.2}$ nanoparticles; this catalyst is developed to selectively produce propanol (C_3H_7OH faradic efficiency is 35.3%). A parametric study is conducted to study design and operating parameters of batch-cell including boundary layer thickness, catalyst layer thickness, catalyst layer porosity, electrolyte nature, and strength of an electrolyte at a fixed applied cathodic voltage of -1.0 V vs RHE. Numerical model is extended to include other working electrodes such as solid electrode (SE), and gas diffusion layer electrode (GDLE) to study their effect on total current density (TCD).

10:40 AM

Breaking Frontiers in Selective Electroreduction of CO2 to Ethylene Under Controlled Catalyst Regeneration

Nitin Minocha, PhD, Meenesh R. Singh
(Department of Chemical Engineering,
University of Illinois, Chicago)

Electrochemical reduction of CO_2 (ECR) powered by renewable energy sources have emerged as a powerful technology to fight a global battle against climate change. Considering the huge industrial importance (global market size of $230 billion) of ethylene and its contribution towards CO_2 emission (~150 Mt of CO_2 emission per year), it is necessary to find sustainable methods for synthesizing ethylene. Therefore, this work focus on breaking frontiers in electrochemical reduction of CO_2 to ethylene with higher product selectivity, high current density and long-term stability. The experimental results reveal that in case of continuous reduction HER (FE = 70%) is dominating at all current densities. In order to improve the selectivity towards multicarbon products, a methodology is developed for catalyst regeneration under controlled microenvironments by applying oscillating reduction and oxidation currents. The experimental results reveal that reduction current (I_R) and oxidation time (t_O) are the important parameters affecting the performance of electrochemical cell. Once the catalyst regeneration is ensured, the electrolyzer design is further optimized to attain higher selectivity. The factors under consideration are 1) Flow configuration; (2) Catalyst location; (3) Improve hydrodynamics for bubble clearance; (4) Process parameters and (5) the strategy to attain target potential. The experimental results clearly demonstrate that the selectivity is highly dependent upon these parameters. The crossflow configuration favors methane (FE = 44%), whereas flow by configuration shows 50 % FE towards ethylene and ethanol. This behavior is attributed to the formation of Cu (I) oxides for flow by configuration which leads to higher affinity towards C2 products.

11:05 AM

Electrochemical One-Pot Systems for Advancing Carbon Capture and Utilization in Simulated Flue Gas Conditions

Rohan Sartape, Vamsi V. Gande, Meenesh R. Singh
(Department of Chemical Engineering,
University of Illinois, Chicago)

The rising concerns of global boiling due to the accumulation of CO_2 and associated disruption to the flora and fauna caused by fossil-fuel-based emissions necessitate an urgent development of CO_2 sequestration and utilization systems. An electrochemical one-pot system for carbon capture and utilization is an attractive avenue to investigate as it can avoid the costs, space, and risks of the transportation of compressed CO_2 while producing value-added fuels from renewable energy. Moreover, tuning such systems to synthesize C_2 products is economically feasible. Herein, we demonstrate the development of an electrochemical one-pot system synthesizing C_2 product with Faradaic Efficiency of up to 80% under simulated flue gas conditions. To leverage an optimal performance from the system, we also study the effects of different parameters such as the type of catalyst, electrolyte concentration, percentage of CO_2 in feed, gas contact time, gas feeding conditions, and applied voltage. Finally, we demonstrate a long-term stability experiment to validate the feasibility of the process for the real-world applications.

Tuesday Afternoon Keynote Session

12:45 PM

Status of Batteries for Transportation and Grid Decarbonization

Venkat Srinivasan, Director of the Argonne
Collaborative Center for Energy Storage Science,
Argonne National Laboratory

Track 1
Energy Storage II

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

2:00 PM

Assessing Particle Degradation in Thermochemical Energy Storage through Imaging

Spenser Vasich (Mechanical Engineering, Michigan State University, East Lansing, MI)

Thermochemical energy storage is an important emerging topic in the energy space. The ability to store renewable energy in a thermochemical form allows for a more consistent energy system on which to rely and reduces greenhouse emissions.
Many thermochemical particle systems utilize a moving bed oxidation reactor with magnesium-manganese-oxide pellets to store and release energy via a renewable energy source. However, the magnesium-manganese-oxide pellets' re-useable nature presents an issue, as these particles experience degradation as they are subject to particle-particle contact and contact with the surfaces of the reactor chamber. Understanding how much attrition these particles are incurring is paramount, as a larger industrial operation could experience efficiency and functionality issues if the particles were to degrade substantially.
To find the degree to which particles experience wear, this work describes a real-time imaging system for evaluating particle size. In the proposed system, a mounted camera utilizes ImageJ and its macro code to autonomously analyze the area of 100 particles at a time strewn across a 10x10 mesh. Measuring the level of attrition occurring involves finding the average area of a sample of 1000 particles from the initial batch, running those particles through the reactor 9 times, each time measuring another sample. Given that particle attrition can be quantified by the change in the average area of the particles, the overall decrease in the average area between the initial and final sample can be used to conclude the level of attrition experienced by the particles in the reactor for each run.

2:25 PM

Upgrading Sustainable Materials into Specialized Flow Battery Chemistries

Patrick Sullivan (Flux XII Inc., Madison, WI)

Flux XII Inc. upgrades organic feedstocks into specialized flow battery chemistries for grid energy storage. After experimentally screening hundreds of organic redox structures, we have demonstrated record lab-scale performance, produced ton-scale batch reactions, and are testing kW prototypes. This talk will tell the startup's story of developing the fundamental technology at the University of Wisconsin-Madison and our vision for storing clean energy in sustainable materials. Come hear about potential job openings and partnership opportunities with Flux.

2:50 PM
Negative Electrodes Performance of Lead-Acid Batteries: Analysis from Modeling Cyclic Voltammetry Responses
Mohammed Effat (Chemical Sciences and Engineering, Argonne National Laboratory, Lemont, IL),
Kevin Knehr (Argonne National Laboratory, Lemont, IL)
Crystal Ferels (Argonne National Laboratory)
Chaudhari Nikhil (Argonne National Laboratory)
Pietro Lopes (Material Science Department, Argonne National Laboratory)
Tim Fister (Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL)

Lead-acid batteries (LABs) play a key role in the energy storage sector with applications spanning from starting-ignition-lightning batteries to grid energy storage. Passivation of lead negative electrodes by PbSO4 crystals is a one fundamental mechanism limiting the performance of LAB. In this regard, we developed an electrochemical mathematical model that simulates the nucleation and growth dynamics of PbSO4 crystals on a flat lead electrode, responsible for its passivation. The model considers the electrochemical dissolution of lead electrode and the transport of species in the H2SO4 electrolyte. We have compared the model predictions with a rich dataset of cyclic voltammetry (CV) responses collected at several scan rates and several concentrations of H2SO4. The model shows a good agreement with the experimental data including the onset potential, center, height, and width of the CV peaks, and discharge capacity. The model is used to give insights on how acid concentration influence the electrochemical response of lead negative electrodes.

Track 2
Process Safety I

Chair: Jessica Morris (BakerRisk)
Co-Chair: Zac Adesanya (UIC)

2:00 PM
Important Characteristics of an Effective Process Safety Knowledge Management System
Tekin Kunt (PSRG Inc., Houston, TX), Anthony Do (PSRG, Inc., Houston, TX)

Process Safety Knowledge Management (PSKM) System is a platform to convert data to information, information to knowledge, and knowledge to wisdom. An effective PSKM System allows an organization to capture, organize, maintain, and provide the right Process Safety Knowledge (which also includes Process Safety Information) to the right people at the right time to improve its process safety performance.
Data is a specific piece of information, such as the relief setting on a pressure relief device. Information is a grouping of data items and a description of their interrelationships such as Cause-Consequence scenarios. Knowledge is the assimilation of information into the human component of an organization, for example, when an operator knows a particular operating procedure. Wisdom is the application of knowledge as a deeper capability leading to competency and enhanced expertise yielding an exceptional value. Wisdom is the applied experience that is often not retained in an organization as people age out and retire.
In this talk, we will introduce the key characteristics of an effective PSKM System. The talk will conclude with examples of implementation from Chemical Processing Industries.

2:25 PM
Process Safety of Combustible Dust, the Dust Hazard Analysis
Danielle Kittaka, Timothy Cullina (Risk Management, Fauske and Associates, Burr Ridge, IL

This presentation will discuss an approach to identify, assess, and eliminate/control dust explosion hazards in facilities. This presentation will discuss why dust explodes and how to screen the raw, intermediate, and final process materials and wastes that facilities handle to determine the precautions that should be taken in handling, processing, and storing combustible particulates. This will include sensitivity to various types of ignition sources - such as electrostatic discharges, hot surfaces, open flames, mechanical sparks, hot work, etc., - and the severity of combustion incidents - such as explosions and flashfires.

Combustible dusts are a recognized hazard for industrial facilities everywhere and performing a dust hazard analysis (DHA) is an important tool to evaluate your risk of an explosion and flashfire. This presentation will include information the “Dust Hazard Assessment (DHA)” requirements of the National Fire Protection Association (NFPA) 652: Standard on Fundamentals of Combustible Dusts.
This presentation provides a starting point for completing a DHA from identifying and assessing combustible dust and its hazards to process equipment review and recognition of retroactively required management programs. The workshop will clarify the relationship between the shared fundamentals standard and the industry-specific standards such as NFPA 484 for metals, NFPA 654 for chemicals, plastics, and pharmaceuticals, NFPA 664 for wood, NFPA 655 for sulfur, and NFPA 61 for agricultural and food processing. These standards require that a facility processing or handling combustible dust perform a hazard analysis for affected each operation.

2:50 PM

Hazardous Waste Generators and Treatment Facilities: Hazardous Waste Characteristics, Rcra, and Treatment Technologies

Trevor Lardinois (Exponent Inc, Warrenville, IL), Brenton Cox (Thermal Sciences, Exponent, Inc., Warrenville, IL)

The United States Environmental Protection Agency implemented the Resource Conservation and Recovery Act (RCRA) in 1976, which created a framework for the comprehensive management of hazardous waste. Hazardous waste is waste that is dangerous or capable of imposing harmful effects on human health or the environment. RCRA provides guidelines on how to manage hazardous waste from the point of generation until its ultimate disposal (i.e., cradle-to-grave). The RCRA regulations impose different responsibilities on hazardous waste generators and treatment storage and disposal facilities (TSDFs) to facilitate the safe disposal of hazardous waste. Another technical aspect of hazardous waste management is the characterization of complex waste streams and the associated hazards. This presentation will introduce the relationship between generators and TSDFs, while focusing on RCRA regulations and concepts of hazardous waste management from cradle to grave. Additionally, various case studies will be used as examples to illustrate when mismanagement leads to catastrophe.

Track 1
Fluid Properties, Fluid Dynamics & Transport Phenomena

Chair: Hadjira Iddir (Honeywell UOP)
Co-Chair: Paul Vesely (Spraying Systems Co.)

3:30 PM

Prediction of Densities in Fluidized Bed Strippers for Various Types of Internals

Allan Issangya (Particulate Solid Research, Inc. (PSRI), Chicago, IL)
Surya Karri (Particulate Solid Research, Inc., Chicago, IL)

King (1989) developed a correlation for calculating the overall bed voidage for FCC catalyst particles in gas-solids fluidized beds. The correlation is based on the two-phase theory and incorporates simplifying assumptions obtained from apparent bulk density data of 16 commercial equilibrium catalysts and from bed density measurements in commercial FCC beds that included 9.1 and 16 m (30 and 52 ft) diameter fluidized bed regenerators and 3, 3.7 and 4.6 m (10, 12 and 15 ft) diameter fluidized bed strippers. While the above correlation is very useful for interpolation and quantitative assessment, it is not easily generalizable or intuitive. We developed an intuitive modification to King’s equation, for enhancing qualitative—and hopefully quantitative—understanding. King’s equation was mostly developed for the case of zero net solids flux in the fluidized bed . We postulate that imposing a downward solids flux increases the effective volumetric flux of gas against the solids. This paper compares the bed density predictions of the original King's correlation and it's modified version to our experimental FCC catalyst data measured in a 0.9-m (3-ft)-diameter fluidized bed stripper unit operated with three types of stripper internals: grating trays, cross-hatched sheds and disk and donut trays at three superficial gas velocities and various solids fluxes.

3:55 PM

Using Network Theory to Gain Novel Insights on Flow and Dynamics of Dense Suspensions: Node and Edge Centric Methods

Alessandro d'Amico (Chemical & Biomolecular Engineering, Case Western Reserve University, Cleveland, OH) Sidong Tu (Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, OH), Abhinendra Singh (Case Western Reserve University)

Dense suspensions of neutrally buoyant particles, at high packing fraction, ϕ display high non-intuitive non-newtonian flow properties, such shear-thickening or shear jamming[1,2]. Recent simulations have been successful in quantitatively reproducing experiments through Lubrication-Friction Discrete Element Method (LF-DEM) models where particles interact via hydrodynamic lubrication forces and frictional contact forces[3,4,5]. This picture is still mean-field and the collective motion of particles and in depth study of mesoscale contact and force network that is continuously formed and destroyed under shear is still poorly understood. Here we use network theory to provide insights into detailed mesoscale features using two dimensional simulations of shear thickening suspensions. An edge centric approach to network theory indicates that at low stresses, when the network is not fully developed the third order loop edges are the major contributing factors in describing the strong shear thickening behavior. Additionally, a node centric approach reveals that as networks fully develop, the average angle between nodes decreases. Our results highlight the critical importance of mesoscale collective motion and rearrangements, thus providing a new way to understand the flow behavior of dense suspensions.

Track 2
Process Safety II

Chair: Jessica Morris (BakerRisk)
Co-Chair: Zac Adesanya (UIC)

3:30 PM

Hazardous Area Classification Best Practices

Calvin Doty (BakerRisk)

The objective of Hazardous Area Classification (HAC) is to identify and classify a 3-dimensional space that contains flammable / combustible materials and electrical equipment in order to minimize uncontrolled ignition of flammable material from an electrical source. Many industrial standards address HAC, such as NFPA 497, API RP 500, and IEC 60079-10-1, and each criterion differs in their approach and details. Using these codes, potential release sources are classified based on the type of flammable hazard, the frequency at which the flammable hazard is present, and the fire hazard properties of the material. Based on these criteria, HAC contours can be developed around release sources based on the HAC guidance standard. Electrical equipment within those HAC contours should adhere to the specified HAC classification minimize the potential of an accidental ignition of a released flammable material. The presentation will dive into HAC basics and logistics emphasizing the importance of HAC as well as a review of BakerRisk's Scenario-Based HAC methodology and its comparison to the traditional Unit Boundary HAC methodology.

3:55 PM

Shelter-in-Place Guidance/Best Practices to Tackle Toxic Exposure

Sajjid Odeh, Jessica M. Morris, and Anthony Sarrack (BakerRisk)

Emergency response planning is required by PSM in accordance with 29 CFR 1910.38, but what should really be considered in the case of a toxic release emergency? While Shelter-in-Place (SIP) is an efficient strategy to protect on-site personnel from a toxic release, many elements and complexities need to be taken into consideration when planning an SIP strategy. Developing an efficient strategy can be challenging as there is no single standard or recommended practice that outlines a comprehensive approach for sheltering in place due to toxic exposure. This presentation will cover best practices for Shelter-in-Place across multiple processing facilities. This holistic approach recognizes the need for reliable detection, time response (isolation, ventilation, etc.), design principles to minimize ingress of hazardous vapors, training, and fallback plan to evacuate if the SIP is compromised.

Poster Session

Characterizing and Engineering Homologs of a Template-Independent DNA Polymerase for Signal Recording Applications

***Teresa Rojas Rodríguez**, Marija Milisavljevic and Keith Tyo,* (Northwestern University)

Measuring cellular signals is essential for understanding complex biological systems. DNA-based recording offers the potential for less invasive and higher-throughput methods, as DNA is a high-density information storage medium deployable in cells. However, existing DNA recorders rely on signal-induced expression of DNA-editing enzymes for signal transduction, which occurs at slower timescales and prevents recording of sub-hour signals. Recently, temporal recording of environmental signals at minute resolution was demonstrated in vitro using terminal deoxynucleotidyl transferase (TdT), a template-independent polymerase. TdT adds deoxyribonucleotides (dNTPs) to the 3' end of single stranded DNA (ssDNA) and changes dNTP preference depending on environmental conditions; signals are therefore encoded in the composition of TdT-synthesized ssDNA. However, TdT is inhibited by ribonucleotide presence (abundant in cellular environments), shows minimal response to some signals of interest, and exhibits slower incorporation rates compared to replicative polymerases. To overcome these limitations through protein engineering, understanding TdT sequence-structure-function relationships is necessary. To explore these relationships, we characterized diverse natural TdT homologs, assessing catalytic activity, responsiveness to cation signals, and activity in the presence of ribonucleotides. Certain homologs exhibit higher responses to cations in vitro, and multiple sequence alignment of TdT sequences revealed shared amino acid identity at specific residues common to more responsive homologs. We introduced equivalent point mutations in a low-response homolog to understand the effects of altering these non-conserved TdT regions. This new knowledge can guide targeted protein engineering efforts to optimize TdT as a recording tool.

Quantum Mechanical Modeling of Enzyme Promiscuity: Application to Carboligases

Geoffrey Bonnanzio (Northwestern University)

Enzyme promiscuity is the tendency of an enzyme to catalyze reactions similar to, yet distinct from, their native reactions. Understanding the extent of reaction promiscuity an enzyme is capable of can enable their use as novel biocatalysts to synthesize complex chemicals, fuels, and pharmaceuticals using new-to-nature reactions. While traditional methods to predict the extent of an enzyme's activity rely on the chemical similarity of reactants, protein structure and biophysics is often missed. Recent advances in protein structure prediction have enabled us to model reactions directly within the enzyme active site. By modeling the reaction with quantum mechanical methods, such as density functional theory, a more detailed insight into the reaction thermodynamics can be achieved in order to better predict the feasibility of new-to-nature reactions. The current work focuses on understanding the range of substrates compatible with carboligases, a class of carbon-carbon bond forming enzymes. Specifically, we model a condensation reaction of two a-keto acids to produce a-hydroxyketone, a useful building block for the pharmaceutical industry.

Process Design, Scaling, and Integration of Catalytic Reactor and Separation Sections for Dehydration of Lactic Acid to Acrylic Acid

***Christopher P. Nicholas**, *Zac Pursell** (Låkril Technologies Corporation)

Acrylic acid and the four primary acrylate derivatives are the cornerstone of a $10B market with broad application across super-absorbent polymers, paints, coatings, and adhesives industries. Producing these chemicals necessary for modern life from sustainable pathways is of key interest. We focus on the dehydrative conversion of feeds derived from lactic acid, a product sustainably fermented from a range of bio-derived sugar sources, to yield acrylic acid.
Lakril Technologies uses zeolite based catalyst formulations where engineered additives such as an amine help control Bronsted acidity and can provide desirable selectivity tuning. Additives 1,2-bis(4-pyridyl)ethane (12BPE) and 4,4-trimethylenedipyridine (44TMDP), at a nominal loading of two molecules per

Na-FAU supercage, afforded a dehydration selectivity of 96±3% over 2000 min time on stream, exceeding the commercial viability target for selectivity of 90%. Tuning the weight hourly space velocity (WHSV) from 0.9 to 0.2 h-1 afforded a yield as high as 92% at a selectivity of 96% with 44TMDP impregnated Na-FAU, resulting in the highest yield reported to date.

Commercial production requires scaled up catalyst and integrated reaction and separation processes. We present here our latest results on process design, scaling, and the integration of catalytic reaction and separation sections for the dehydration of lactic acid to acrylic acid.

Tuesday Dinner Keynote

6:30 PM
Leadership, Innovation, and the Pursuit of Legacy. From Chemical Engineer to FORTRESS Protective Buildings
Karen Vilas **(**President, FORTRESS Protective Buildings)

Presentation Abstracts (Day 2)

Wednesday, March 6, 2024

Wednesday Morning Keynote Session

8:35 AM

First principles treatments of heterogeneous electrocatalysis – reactivity trends and electrocatalyst structure

Jeff Greeley (Purdue University)

Advances in the theoretical understanding of electrochemical systems have, over the past decade, led to growing use of periodic Density Functional Theory studies to treat a surprisingly large ensemble of electrocatalytic reactions, ranging from carbon dioxide electroreduction to oxygen evolution. Many such studies have employed simplified models of the electrochemical environment to determine reactivity trends across a broad space of catalytic materials, while other efforts have focused on developing detailed descriptions of electrochemical phenomena, such as the structure of electrochemical double layers, on model catalyst structures. An emerging challenge is to combine these approaches to ultimately enable theoretical design of electrocatalysts for reactions of significantly expanded chemical and materials complexity.

In this talk, I will begin by discussing how we have applied strategies from computational heterogeneous catalysis to design enhanced electrocatalysts for the classic oxygen reduction reaction. I will then explore challenges in obtaining more detailed descriptions of the electrocatalytic reaction environment, including the structure of catalysts with solid/solid interfaces, the distribution of charges in electrochemical double layers, and the structure and entropy of solvents near the electrocatalyst surface. I will conclude with some perspectives on how these complexities may be incorporated into traditional computational catalyst screening approaches to identify improved materials for more complex electrocatalytic *systems.*

Track 1 – Advances in Refining / Materials

Chair: *Jason Wu* (Honeywell UOP)
Co-Chair: *Nick Shulman* (Exponent)

9:50 AM

Integration of reconciliation infrastructure for refinery scheduling model tuning

Sean R. Werner, PhD
(Blending and Scheduling Improvement Engineer ExxonMobil Technology and Engineering Company - EMTEC)

ExxonMobil and AspenTech have recently co-developed a new refinery scheduling model within Aspen Petroleum Scheduler (APS). A significant technical requirement included building a model reconciliation infrastructure to ensure each refinery unit submodel can accurately predict product yields within a reasonable tolerance. The infrastructure includes “reconciliation events”, containing actual unit feed rates and operating conditions, and special logic units that direct reconciled data to each refinery unit submodel. The reconciliation enables comparisons between predicted product and actual yields that can be used to identify model bias adjustments. An example of how this infrastructure was used to improve distillate hydrotreater model prediction accuracy will be presented.

10:20 AM

Metal-Organic Frameworks at Numat™: A Decade of Innovation, High-Tech Manufacturing, and Future Growth.
William Morris (NuMat, Chicago, IL)

Over the past decade, Numat™ has focused on commercializing metal-organic frameworks (MOFs). To facilitate the commercialization of MOFs, Numat has expanded its team to over eighty individuals with expertise in chemistry, engineering, business development, manufacturing, and quality. Concentrating on applications characterized by small volumes and high value, Numat has successfully brought MOF products to market, catering to the defense and electronics industries. In 2024, Numat announced a transition to a new domestic manufacturing site with the capacity to produce two hundred tons of MOF-based products annually. This presentation will offer a historical perspective on Numat's growth, highlight the new Chicago-based manufacturing site, and provide a perspective on growth areas.

10:50 AM

Petrochemical Transformation: Overcoming Challenges in the Olefins Industry with Naphtha to Ethane/Propane (NEP) Technology
***Robert Szczesniak**, Greg Funk* (Honeywell UOP)

The olefins industry confronts a range of challenges, including growing concerns on the price and supply of certain feedstocks and the need to become more sustainable. While ethane remains the most economical option for ethylene production, its availability is regional with the Middle East and North America having the greatest supply. Significant investments in steam cracking and ethane export facilities in North America have been made over the past decade leading to some forecasts predicting a future increase in the price of ethane. Given the high cost to transport ethane, this poses a particular threat to steam cracking operators in Europe and Asia that have become reliant on imported ethane.

To address these issues, the Naphtha to Ethane/Propane (NEP) technology emerges as a versatile solution to produce a tunable amount of ethane and propane from naphtha and/or LPG. The ethane from NEP is typically fed to an ethane cracker to produce the target amount of ethylene. Propane can be fed to a propane dehydrogenation unit to produce the desired amount of propylene. Compared to a mixed-feed steam cracker, a typical NEP-based olefins complex increases olefin yield by more than 40%, while also reducing cash cost of production, CAPEX per ton of olefin, and CO2 per ton of olefin.

Track 2 – Bioengineering and Nanotechnologies

Chair: *Meltem Demirtas* (Argonne National Laboratory)
Co-Chair: *Wujie Zhang* (Milwaukee School of Engineering)

9:50 AM

Long-Term Antibody Release Polycaprolactone Capsule and the Release Kinetics in Natural and Accelerated Degradation
***TJ Waterkotte**[1], Xingyu He[2], Apipa Wanasthop[3], S. Kevin Li[3] and Yoonjee Park[4]*
([1]Chemical & Environmental Engineering, University of Cincinnati, Cincinnati, OH, [2]University of Cincinnati, Cincinnati, OH, [3]University of Cincinnati, [4]Biomedical, Chemical & Environmental Engineering, University of Cincinnati, Cincinnati, OH)

Although therapy using monoclonal antibodies (mAbs) has been steadily successful over the last 20 years, the means of delivery of mAbs has not been optimized, especially for long-term delivery. Frequent injections or infusions have been current standard of care. In this study, we have developed a long-term antibody biodegradable implant using a porous polycaprolactone (PCL) capsule. It released Bevacizumab (Bev) slowly for 8 months to date. The Bev release kinetics fit a drug release model with experimental data of the diffusion coefficient and partition coefficient through the polymer capsule. Since screening drug release profiles for the long-term (> 6 months) is time consuming, an accelerated degradation method was used after validating characteristics of the PCL capsule in natural and accelerated degradation conditions. The correlation of time period between the natural and the accelerated degradation was determined. Overall, the study suggests mAbs can be released from a porous PCL capsule without an effect of the polymer degradation over the long period (~ 6 months) and the long-term release kinetics can be determined by the accelerated degradation within 14 days.

10:20 AM

High-Throughput Screening of *E. coli* Ghosts Against 314 G-Protein Coupled Receptors (GPCRs)

***Christopher Vidmar*[1]** *and Jennifer Fiegel*[2]
([1]University of Iowa, Iowa City, IA, [2]Department of Chemical and Biochemical Engineering / Department of Pharmaceutical Sciences and Experimental Therapeutics, University of Iowa, Iowa City, IA)

Bacteria display surface components that can interact with receptors found within the body. These interactions can act as anchor points to avoid clearance, facilitate internalization, or regulate an immune response by hijacking receptor signaling. Bacterial surface components are known to interact with G-protein coupled receptors (GPCRs), a class of transmembrane receptors that are often overexpressed in certain disease conditions. We hypothesize that by exploiting these bacteria-GPCR interactions, we can develop more effective drug delivery vehicles. However, identifying these interactions has traditionally been a slow and expensive process since only one receptor-ligand pair could be investigated at a time. Our approach is to produce bacterial ghosts that will allow us to use high-throughput screening techniques to explore interactions between bacterial surface components and hundreds of GPCRs. Ghost bacteria are non-living bacterial cells devoid of their internal components with a fully intact membrane. This project ultimately aims to use these bacterial ghosts as a drug delivery vehicle targeting GPCRs. Bacterial ghosts were produced by treating a commensal *E. coli* strain with calcium carbonate, sodium dodecyl sulfate, sodium hydroxide, and hydrogen peroxide. Successful production was confirmed by measuring DNA release, staining the membrane with crystal violet, and imaging the intact membrane with SEM. Interactions between ghost *E. coli* and 314 GPCRs were then explored using the high-throughput screening technique, PRESTO-Tango. This screening identified interactions that overlap with known bacteria-host pathways and identified unexplored interactions. Current work is dedicated to validating initial hits, producing bacterial ghosts from other *E. coli* strains, and drug loading.

10:50 AM

A Wide Look at MXene-based CO2 Reduction Electrocatalysts: Pioneering Pathways for Green Formaldehyde Production

***Sixbert P. Muhoza*[1]** *Shiba P. Adhikari*[1] *Francisco Lagunas Vargas*[1]*, Anupma Thakur*[2]*, Songge Yang*[3]*, Yu Zhong*[3]*, Babak Anasori*[2]*,and Zachary D. Hood*[1]
([1]Applied Materials Division, Argonne National Laboratory, Lemont, IL, [2]School of Materials Engineering, Purdue University, West Lafayette, IN, [3]Materials Science and Engineering, Worcester Polytechnic Institute, Worcester, MA)

Transition metal carbides, oxy-carbides, nitrides, and carbonitrides (MXenes) constitute an ever-growing class of two-dimensional materials with unique properties, including high conductivity and surface area as well as versatile and tunable surface chemistry. Such a wide-ranging array of properties primes MXenes for various applications and, hence, provides them with the potential to tackle some of the most pressing challenges faced by our planet. Climate change is one such challenge, and the electrochemical CO2 reduction reaction (CO2RR) provides a potent pathway to alleviate the effects of CO2 emission on the environment. The maturation of electrochemical CO2RR, however, will require the development of electrocatalysts that maximize the value gained from converting the CO2 feedstock. For this reason, we have developed a novel class of MXene-based electrocatalysts that leverage the unique properties of MXenes to convert CO2 to formaldehyde. Formaldehyde is a key ingredient in manufacturing many value added products, including resins, coatings, and vehicle components. However, formaldehyde is not typically generated with traditional electrocatalysts, indicating that the herein introduced MXene catalysts drive CO2RR through new reaction pathways. This work highlights the behavior of a wide array of MXenes: ranging from single-layered traditional MXenes to multi-layered MXene/metal heterostructures. The Ti3C2Tx/Cu-M heterostructures were developed through a novel electroless deposition of the bimetals onto the surface of MXenes by oxidizing the Ti moieties of the Ti3C2Tx MXene. The reduction potential of the adsorbed metals dictated this process, with the strongly oxidizing metals reaching their lowest oxidation states while the weakly oxidizing metals were only partially reduced. In all cases, formaldehyde was generated and the highest efficiencies were achieved at low, industrially relevant, cell potentials (between -1.4 V to -2.2 V). These results, as they pertain to pioneering green formaldehyde production and favorability for industry adoption, warrant further exploration of the MXene-based CO2RR electrocatalysts.

Afternoon Keynote

12:45 PM Keynote Introduction

Jason Wu (Programming Chair, Honeywell UOP)

12:50 PM

Nitrogen Electrochemistry to Support DOE's Energy Earthshots

Meenesh Singh (Professor, Department of Chemical Engineering, University of Illinois at Chicago)

As the global climate crisis escalates and the transition to a sustainable energy economy crystallizes, the capability for long-term grid-scale storage and conversion of carbon-free energy remains an unmet challenge. Given the intermittent nature of sustainable energy sources, a global phase-out of greenhouse gas-intensive energy sources will require efficient storage and conversion of sustainable energy. In particular, interest is growing in the interconversion of dinitrogen (N_2) and ammonia (NH_3), given the high energy density of NH_3 (~6.25 kWh kg^{-1}). Apart from being a critical fertilizer component, NH_3 is also an ideal hydrogen carrier (17.7 wt%, 40% higher than methanol), and can be readily transported and stored using existing infrastructures and then directly utilized for energy applications such as a direct ammonia fuel cell (DAFC). However, today most NH_3 is synthesized via the century-old Haber-Bosch process, which operates at extreme temperature (723-823K) and pressure (250-350 atm). It is estimated that NH_3 synthesis consumes about 1% of the world's electricity and a significant fraction of the world's natural gas for hydrogen production via steam reforming of methane. Electrochemical synthesis of NH_3 from N_2 at near-ambient conditions would allow a drastically reduced carbon footprint while simultaneously enabling carbon-free energy storage. The electrochemical N_2 reduction reaction (N2RR) is unfortunately hindered by competition with the hydrogen evolution reaction (HER); as a result, despite years of efforts and significant capability and knowledge advances, state-of-the-art N2RR catalysts yield NH_3 on the order of μA cm^{-2}, orders of magnitude lower than the DOE REFUEL target of 300 mA cm^{-2}. This talk will address the critical need to identify possible alternative routes towards interconversion of N_2 and NH_3. In the absence of such a capability, a transition to a sustainable energy portfolio will face serious challenges.

Track 1 – Machine Learning / Optimization I

Chair: *Mohammed Effat* (Argonne National Laboratory)

Co-Chair: *David Neira* (Purdue University)

2:00 PM

Early Detection of Catalyst Transfer Pipe Plugging Using Temperature Signal Analysis

Holly Butcher*, Mahesh Kumar Gellbaoina, and* ***Louis Lattanzio***

(Honeywell UOP)

This work presents an algorithm for early detection of catalyst transfer pipe plugging in Oleflex processes which continuously monitors temperature signals from skin thermocouples. Utilizing adaptive reference parameters that update in real-time based on process variables, the algorithm proactively identifies anomalies indicative of potential plugging, enabling timely corrective actions to prevent costly unplanned shutdowns and production losses, ultimately enhancing process reliability and operational efficiency.

2:25 PM

Importance Learning Analysis of Ethylene Polymerization By a Single-Atom Cr/SiO_2Catalyst

Changhae Andrew Kim[1]*, Armin Shayesteh Zadeh*[1] *and Baron Peters*[1,2]
([1]Chemical and Biomolecular Engineering, University of Illinois Urbana-Champaign, Urbana, IL, [2]Chemistry, University of Illinois Urbana-Champaign, Urbana, IL)

Despite its industrial relevance, many aspects of Cr/SiO_2 remain enigmatic: (i) the amorphous structure of SiO_2 entails an unknown quenched disorder, (ii) the Cr atoms exhibit different affinities and activities at different surface sites, and (iii) a small number of active sites dictate the catalytic activity. We use the importance learning algorithm to investigate the structural heterogeneities of the single-atom Cr/SiO_2 catalyst. The algorithm combines kernel regression and importance sampling, iteratively generating predictions of site-specific and site-averaged properties from calculations on hundreds of sites. We identify the most active sites and find that they exhibit diffusion-controlled polymerization kinetics in the polymer melt. Further, we observed a trade-off between the grafting affinity and the catalytic activity that is tuned by the strain in the surface site structure.

2:50 PM

Logic-Based Discrete-Steepest Descent: A Solution Method for Process Synthesis Generalized Disjunctive Programs

Albert Lee[1]*, Daniel Ovalle*[2]*, David Alejandro Linan Romero*[3] *Luis Ricardez-Sandoval*[4]*, Jorge M. Gomez*[5]*, Ignacio Grossmann*[2] *and David E. Bernal Neira*[6]
([1]Chemical Engineering, Purdue University, West Lafayette, IN, [2]Chemical Engineering Department, Carnegie Mellon University, Pittsburgh, PA, [3]University of Waterloo, Waterloo, ON, Canada, [4]Chemical Engineering, University of Waterloo, Waterloo, ON, Canada, [5]Chemical Engineering, Universidad de los Andes, Bogotá, Colombia, [6]Quantum Artificial Intelligence Laboratory, NASA Ames Research Center, Moffett field, CA)

The optimization of chemical processes is challenging because of the non-linearities and discrete decisions involved. In particular, the optimal synthesis and design of chemical processes can be formulated with Generalized Disjunctive Programming (GDP) in order to optimize the corresponding superstructure of design alternatives. Although several solution approaches are available to tackle these problems, for instance, by reformulating them as Mixed-Integer Nonlinear Programming (MINLP) problems or by applying logic-based algorithms to solve the GDP problem directly, taking advantage of its structure, these methods are still scarce. This study presents the logic-based discrete-steepest descent algorithm (LD-SDA) for optimizing GDP problems involving ordered Boolean variables. The LD-SDA reformulates ordered Boolean variables in GDP problems into integer decisions called external variables. Then, LD-SDA solves the reformulated GDP problem using an upper-level subproblem decomposition that optimizes external variables in the upper-level problem and the remaining continuous and discrete variables in subproblems, only involving those constraints relevant to the external variable considered, taking advantage in this way of the structure of the GDP problem. The advantages of LD-SDA are illustrated through an illustrative batch processing case study, a reactor superstructure, a distillation column, and a catalytic distillation column. We describe an open-source implementation that automatically detects ordered Boolean variables in GDP problems formulated under the Pyomo. GDP modeling paradigm, reformulating and solving the problem according to the LD-SDA. The results show improvements in computational efficiency and solution quality compared to other GDP and MINLP solvers.

Track 2 – Catalysis I

Chair: *Aditya Prajapati* (Lawrence Livermore National Lab)
Co-Chair: *Shri Dawande (Motorola Solutions*)

2:00 PM

Highly Selective and Stable Pt-Co Bimetallic Catalysts Prepared By Atomic Layer Deposition for Unsaturated Aldehyde Hydrogenation

Kaiying Wang[1]*, Xiaofeng Wang*[2] *and Xinhua Liang*[1]
([1]Department of Energy, Environmental & Chemical Engineering, Washington University in St. Louis, St. Louis, MO, [2]Department of Chemical and Biochemical Engineering, Missouri University of Science and Technology, Rolla, MO)

Bimetallic catalysts have found extensive use in the selective hydrogenation of unsaturated aldehydes. Yet, the influence of interactions between bimetallic nanoparticles and substrates on catalytic performance remains unexplored. Utilizing atomic layer deposition (ALD) technology, we deposited highly dispersed Pt-Co bimetallic catalysts of precisely controlled size on multi-walled carbon nanotubes (MWCNTs) and γ-Al_2O_3 nanoparticles. The fine-tuned Pt-Co/MWCNTs catalyst demonstrated high selectivity (>90%) and conversion (>90%) to unsaturated alcohols. A series of experiments and density functional theory (DFT) calculations were conducted to investigate the synergistic effects of Pt, Co, and MWCNTs. We found that the interaction between Pt and Co nanoparticles played a crucial role in achieving high selectivity in carbonyl bond (C=O) activation, and the combined effects of Pt-Co and MWCNTs significantly enhanced the activity of the Pt-Co bimetallic catalysts. Furthermore, when γ-Al_2O_3 nanoparticles were used as the substrate, the stability was significantly improved while maintaining an 81.2% selectivity to unsaturated alcohol. This excellent stability was attributed to the strong interaction between the metal nanoparticles and the γ-Al_2O_3 substrate. The bimetallic strategy, based on the synergistic effects demonstrated in this study, can be extended to other metal nanoparticles and supports, and can serve as a universally rational approach for designing and synthesizing effective catalysts for selective hydrogenation reactions.

2:25 PM

DFT Analysis of Surface-Bound Nitrogen Species Under N_2 Plasma Exposure

Chang Yan[1]*, Garam Lee*[1]*, David Go*[2]*, Casey O'Brien*[1]*and William Schneider*[1]
([1]Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN, [2]Aerospace and Mechanical Engineering, University of Notre Dame, Notre Dame, IN)

Non-thermal plasma (NTP)-assisted catalysis has attracted growing attention as an alternative method for nitrogen (N_2) activation by combining reactive chemical environments induced by NTP with catalysts to drive chemical transformations at temperatures at which such reactions are thermally inaccessible.[1,2] Despite the substantial attention given to the plasma-catalytic conversion of N_2, the intermediates, and mechanisms accessed when a catalytic surface is exposed to plasma- activated N_2 are not well understood. Plasma-enhanced N_2 adsorption on various metal surfaces at ambient temperature had been observed. Previous studies attribute this observation to the presence of atomic N that may cause surface distortion or electronic effect.[3] However, the temperature at which species are observed is inconsistent with the assignment to chemisorbed N_2.[4] Characterization of the species accessible under plasma exposure is key to leveraging plasma- catalysis towards desired products. In this work, we use DFT models to compute the structures, vibrational signatures, and potential energy surfaces for the creation or decomposition of potential N-containing adsorbates at various facets of transition metal surfaces. We compare results with observations from polarization-modulation infrared reflection-absorption spectroscopy (PM-IRAS) of polycrystalline metals exposed to nitrogen plasma. Results reveal the generation of metastable nitrogen adsorbates that are inaccessible through thermal routes.

2:50 PM

Process Design, Scaling, and Integration of Catalytic Reactor and Separation Sections for Dehydration of Lactic Acid to Acrylic Acid

Christopher P. Nicholas *and Zac Pursell*
(Lakril Technologies Corporation, Chicago, IL)

Acrylic acid and the four primary acrylate derivatives are the cornerstone of a $10B market with broad application across superabsorbent polymers, paints, coatings, and adhesives industries. Producing these chemicals necessary for modern life from sustainable pathways is of key interest. We focus on the dehydrative conversion of feeds derived from lactic acid, a product sustainably fermented from a range of bio-derived sugar sources, to yield acrylic acid. Lakril Technologies uses zeolite-based catalyst formulations where engineered additives such as an amine help control Bronsted acidity and can provide desirable selectivity tuning. Additives 1,2-bis(4-pyridyl)ethane (12BPE) and 4,4-trimethylenedipyridine (44TMDP), at a nominal loading of two molecules per Na-FAU supercage, afforded a dehydration selectivity of 96±3% over 2000 min time on stream, exceeding the commercial viability target for selectivity of 90%. Tuning the weight hourly space velocity (WHSV) from 0.9 to 0.2 h-1 afforded a yield as high as 92% at a selectivity of 96% with 44TMDP impregnated Na-FAU, resulting in the highest yield reported to date.

Commercial production requires scaled up catalyst and integrated reaction and separation processes. We present here our latest results on process design, scaling, and the integration of catalytic reaction and separation sections for the dehydration of lactic acid to acrylic acid.

Track 1 – Machine Learning / Optimization II

Chair: *Mohammed Effat* (Argonne National Laboratory)
Co-Chair: *David Neira* (Purdue University)

3:30 PM

Optimizing Reverse Electrodialysis Process for Renewable Electricity Generation from Salinity Gradient

Carolina Tristan[1]*, Marcos Fallanza*[2]*, Raquel Ibañez*[2] *and David E. Bernal Neira*[1,3,4]
([1]Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, [2]Department of Chemical and Biomolecular Engineering, University of Cantabria, Santander, Spain, [3]Quantum Artificial Intelligence Laboratory, NASA Ames Research Center, Moffett field, CA, [4]Universities Space Research Association – Research Institute of Advanced Computer Science, Mountain View, CA)

3:55 PM

Graph-Based Representations and Applications to Process Simulation

Yoel Cortes-Pena[1] *and Victor M. Zavala*[2]
([1]DOE Center for Advanced Bioenergy and Bioproducts Innovation, University of Illinois at Urbana-Champaign, Urbana, IL, [2]Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI)

4:20 PM

A Water-Energy-Food Nexus Framework to Improve Resource Security

Brenda Cansino Loeza[1,2], Aurora Del Carmen Munguia Lopez[2], Jose Ponce-Ortega[3] and Victor M. Zavala[2]
([1]Chemical Engineering, University of Wisconsin-Madison, Madison, WI; [2]Department of Chemical and Biological Engineering, University of Wisconsin Madison, Madison, WI, [3]Department of Chemical Engineering, Universidad Michoacana de San Nicolas de Hidalgo, Morelia, MI, Mexico)

Track 2 – Catalysis II

Chair: *Aditya Prajapati* (Lawrence Livermore National Lab)
Co-Chair: *Shri Dawande* (Motorola Solutions)

3:30 PM

Two-Phase Reactors and Population Balance Models for Polymer Upcycling

Changhae Andrew Kim[1], *Chinmay A. Sahasrabudhe*[1], *Yi-Yu Wang*[2], *Ryan Yappert*[1], *Andreas Heyden*[3], *Wenyu Huang*[2,4], *Aaron Sadow*[2,4] *and Baron Peters*[1,5]
[1]Chemical and Biomolecular Engineering, University of Illinois Urbana-Champaign, Urbana, IL, [2]Department of Chemistry, Iowa State University, Ames, IA, [3]Chemical Engineering, University of South Carolina, Columbia, SC, [4]U.S. DOE Ames Laboratory, Ames, IA, [5]Chemistry, University of Illinois Urbana-Champaign, Urbana, IL)

Polymer upcycling efforts attempt to drive selectivity towards high-value liquid hydrocarbons, rather than light gases. In cases where polymer cleavage is affected by a heterogeneous catalyst in the polymer melt, the volatility of products can be exploited to tune selectivity. Specifically, products that partition into the headspace gas will not be further cleaved, since the catalyst resides in the polymer melt. We formulate and solve population balance models of two-phase reactors to quantify the effects of product volatility on the selectivity of polymer upcycling. We incorporated vapor-liquid partition coefficients into population balance equations to describe polymer upcycling in two-phase reactors. The models consist of vapor-liquid equilibrium models and rate equations that can be nondimensionalized and generalized to a wide range of systems, including batch reactors and flow reactors with several different catalysis strategies.

3:55 PM

Structure and Tunable Nature of Heterogenized Molecular Catalysts Developed By Oxidative Grafting

Jacklyn Hall, *Alon Chapovetsky, Uddhav Kanbur, A. Jeremy Kropf, Massimiliano Delferro and David Kaphan*
(Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL)

Surface organometallic chemistry (SOMC) has emerged as a viable route for well-defined catalyst synthesis through the deposition of molecular organometallic precursors onto traditional solid catalyst supports. In this work, the reducible nature of MnO_2 and lithiated $Li_xMn_2O_4$ supports is leveraged for the grafting of nine organometallic precursors spanning the transition metal series (M = V, Fe, Ni, Cu, Zr, Pd, Ag, and Au), facilitated by oxidative chemisorption involving electron transfer to the support. The speciation of the supported metals was investigated through a combination of X-ray absorption and photoelectron spectroscopic characterizations. Results provided that several complexes (M = V, Fe, Ni, Cu, Zr, and Au) form isolated metal ions located on the surface and within interstitial vacancies of the $Li_xMn_2O_4$ structure, while others such as Pd form isolated molecular fragmented species. The catalytic proficiency of the supported metals was further evaluated for the low-temperature oxidation of CO with O_2 as a probe reaction. Screening of the M/MnO_2 ensemble indicated superior CO_2 formation rates of the oxidatively-grafted materials over the pristine MnO_2 support for all metals except for M = Ni and V under the conditions tested (2.6 kPa CO, 7.7 kPa O_2, T = 25 – 50 °C). Overall, this work demonstrates the achievement of isolated metal centers on $Li_xMn_2O_4$ enabled by the oxidative grafting of well-defined molecular precursors – the evaluation of which enables further understanding of the site and surface properties key to their low-temperature oxidation reactivity.

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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) 16th Annual Midwest Regional Conference. AIChE and IIT 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. We encourage you to stay engaged, ask questions, and have fun!

8:45-9:45	**Engineering Expo** (Hermann Hall Gallery Lounge) - Meet with current engineering students and see some of their projects.
9:45-10:00	**Introduction** (Hermann Hall Auditorium) - 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 (Hermann Hall Auditorium) - Learn about how engineers contribute to all aspects of society.
	Team Building Exercise (Hermann Hall Expo Room) - Work with other students to complete a hands-on engineering-related task.
11:30-12:00	**Engineering Lunch** (Hermann Hall Ballroom and Expo Room) - Opportunity for one-on-one discussions with engineering professionals and students.
12:15-12:45	**Keynote Speaker** (Hermann Hall Auditorium) - Marty Gonzalez – Innovation and Technology Principal, BP
12:45-1:30	**Engineering Panel Session** (Hermann Hall Auditorium) - Learn about the day-to-day activities of practicing engineers and engineering students. Time to ask your most burning questions.
1:30	**Optional – Campus tours** (Meet in the Hermann Hall Gallery Lounge) - Tours of IIT are available for groups that request it.

Marty Gonzalez

Dr. Martin R. Gonzalez holds the position of Innovation and Technology Principal within bp's Digital Transformation & Integration organization. In his 28 years with bp, Marty has held individual and team leader positions in applied research, operations, process design, capital projects, and refinery commercial optimization.

Starting at the Amoco Research Center in Naperville, IL, Marty went from pilot plant to commercial plant, working at two refineries over 16 years before returning to lead a global refinery technology support team. Career highlights include a multi-billion-dollar refinery reconfiguration and initiation of a renewable diesel experimentation and modeling program. Leveraging his hands-on experience in process engineering and research, Marty began working digital projects in 2016. His current focus is on AI-based decision intelligence and digital twin technologies for oil production, refining, wind, and electric vehicles.

Marty holds a Bachelor of Science degree in Chemical Engineering from the University of Illinois at Urbana-Champaign. He holds a PhD in Chemical Engineering from the University of Wisconsin – Madison, where he studied heterogenous catalysis under Prof. James A. Dumesic.

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Young Professionals Social

AICHE Young Professionals Social

Join the AICHE YP group for a social hour to meet young Chemical Engineering professionals in the Chicagoland Area

When: Wednesday March 6th at 6 PM
Where: Cork and Kerry at the Park
Address: 3259 S Princeton Ave, Chicago, IL 60616
Questions?: Email yp.aichechicago@gmail.com

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