14th Annual
AIChE Midwest Regional Conference

March 1-2, 2022

https://www.aiche.org/conferences/midwest-regional-conference/2022

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AIChE Global

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Conference Overview

The AIChE Midwest Regional Conference (MRC) continues into its 14th year. Organized by the **AIChE Chicago Local Section** and **AIChE Global**, 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:

- **Stephen Klejst**, *Executive Director of Investigations & Recommendations, U.S. Chemical Safety and Hazard Investigation Board (CSB)*
- **Simona Rollinson,** *Chief Operating Officer, ISACA*
- **Fouad Teymour,** *S.C. Johnson Professor of Chemical Engineering and Director of the Center for Complex Systems and Dynamics, Illinois Institute of Technology*
- **Henrik Rasmussen,** *Vice President of Catalyst and Technology and Managing Director for the Americas, Haldor Topsoe*
- **Manos Mavrikakis**, *Ernest Micek Distinguished Chair, University of Wisconsin-Madison*

The virtual conference contains **16 technical sessions** featuring over **55 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 virtual outreach program features **Kimberly D. Moore** (President & Founder of KDM Engineering) as keynote speaker and includes a virtual networking session where students can interact with practicing engineers.

On behalf of the conference planning committee, we welcome you to the 14th Annual AIChE Midwest Regional Conference and hope you will take advantage of all the opportunities it has to offer.

Matthew Walters
Conference Chair
Senior Engineer, Exponent

Jessica Morris
Conference Co-Chair
Senior Associate, Exponent

Hakim Iddir
Technical Program Chair
Physicist, Argonne National Laboratory

Belma Demirel
Technical Program Co-Chair
Senior Engineer, bp

Program at a Glance (Day 1)

Tuesday, March 1, 2022

8:15 AM – 8:30 AM	**Conference Welcome** (TuI1)
8:30 AM – 9:30 AM	**Morning Keynote** (TuK1) - Stephen Klejst*, Executive Director of Investigations & Recommendations &* Vonzella Vincent*, Chemical Incident Investigator, U.S. Chemical Safety and Hazard Investigation Board (CSB)*
9:30 AM – 9:40 AM	**Break**
9:40 AM – 10:40 AM	**Technical Sessions** - *Process Safety I* (TuA1) - *Polymer Science* (TuA2)
10:40 AM – 10:50 AM	**Break**
10:50 AM – 11:50 AM	**Technical Sessions** - *Process Safety II* (TuB1) - *Bioengineering & Nanotechnologies I* (TuB2)
11:50 AM – 12:45 PM	**Lunch Break**
12:45 PM – 1:45 PM	**Afternoon Keynote** (TuK2) - Simona Rollinson*, Chief Operating Officer, ISACA*
12:30 PM – 2:00 PM	**Networking with High School Outreach Participants** [optional signup]
1:45 PM – 2:00 PM	**Break**
2:00 PM – 3:20 PM	**Technical Sessions** - *Environmental Compliance & Remediation I* (TuC1) - *Bioengineering & Nanotechnologies II* (TuC2)
3:20 PM – 3:30 PM	**Break**
3:30 PM – 4:50 PM	**Technical Sessions** - *Environmental Compliance & Remediation II* (TuD1) - *Machine Learning & Optimization* (TuD2)
4:50 PM – 5:00 PM	**Break**
5:00 PM – 6:00 PM	**Poster Session** (TuP1)
6:00 PM – 6:30 PM	**Networking Break**
6:30 PM – 8:00 PM	**AIChE Chicago March Dinner Meeting** [Zoom signup link]
7:00 PM – 8:00 PM	**Dinner Keynote** (TuK3) - Fouad Teymour*, S.C. Johnson Professor of Chemical Engineering and Director of the Center for Complex Systems and Dynamics, Illinois Institute of Technology*

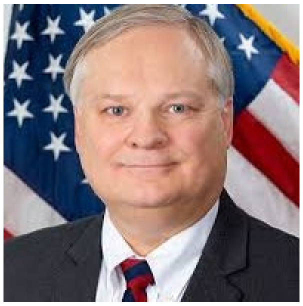
Program at a Glance (Day 2)

Wednesday, March 2, 2022

8:25 AM – 8:30 AM	**Conference Welcome** (WeI1)
8:30 AM – 9:30 AM	**Morning Keynote** (WeK1) - Henrik Rasmussen*, Vice President of Catalyst and Technology and Managing Director for the Americas, Haldor Topsoe*
9:30 AM – 9:40 AM	**Break**
9:40 AM – 11:00 AM	**Technical Sessions** - *Refining & Renewables* (WeA1) - *Climate Solution: Action I* (WeA2)
11:00 AM – 11:10 AM	**Break**
11:10 AM – 12:10 PM	**Technical Sessions** - *Catalysis & Reaction Engineering I* (WeB1) - *Climate Solution: Action II* (WeB2)
12:10 PM – 1:00 PM	**Lunch Break**
1:00 PM – 2:00 PM	**Afternoon Keynote** (WeK2) - Manos Mavrikakis*, Ernest Micek Distinguished Chair, University of Wisconsin-Madison*
2:00 PM – 2:10 PM	**Break**
2:10 PM – 3:30 PM	**Technical Sessions** - *Catalysis & Reaction Engineering II* (WeC1) - *Energy Storage I* (WeC2)
3:30 PM – 3:40 PM	**Break**
3:40 PM – 5:00 PM	**Technical Sessions** - *Fluid Properties, Fluid Dynamics, & Transport Phenomena* (WeD1) - *Energy Storage II* (WeD2)
5:00 PM – 6:00 PM	**Happy Hour**

Keynote Speakers

Tuesday Morning Keynote: 8:30 AM Tuesday, March 1, 2022



Stephen Klejst, *Executive Director of Investigations & Recommendations, U.S. Chemical Safety and Hazard Investigation Board (CSB)*

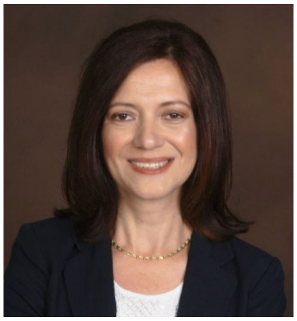
Presentation Title: ***Lessons Learned from the AB Specialty Silicones Explosion and Fire Incident***

Biographical Sketch: *Stephen Klejst, the Executive Director of Investigations and Recommendations, joined the U.S. Chemical Safety Board (CSB) in February 2018. He is responsible for leading the agency's investigation and recommendations programs including the Drivers of Critical Chemical Safety Change advocacy program.* *Stephen Klejst, the Executive Director of Investigations and Recommendations, joined the U.S. Chemical Safety Board (CSB) in February 2018. He is responsible for leading the agency's investigation and recommendations programs including the Drivers of Critical Chemical Safety Change advocacy program.*

Mr. Klejst comes to the CSB after nearly ten years of experience with the National Transportation Safety Board where he was deputy managing director and director of the agency's Office of Railroad, Pipeline and Hazardous Materials Investigations. During his tenure with the NTSB, Mr. Klejst led the agency's investigation of several major pipeline and railroad accidents including the explosion of a natural gas transmission line in San Bruno, California, the rupture of a hazardous liquid transmission line in Marshall, Michigan and several significant freight railroad and transit rail accidents. Prior to joining the NTSB, Mr. Klejst had a distinguished executive career in the railroad industry with responsibilities in the areas of safety, accident investigation, regulatory compliance and technical training.

Mr. Klejst received his bachelor's degree in chemistry from the University of Pennsylvania and a master of science degree in management from the Stevens Institute of Technology. Mr. Klejst is a Certified Safety and Security Director.

Tuesday Afternoon Keynote: 12:45 PM Tuesday, March 1, 2022



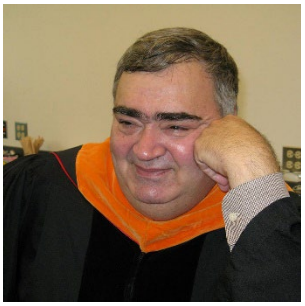
Simona Rollinson, *Chief Operating Officer, ISACA*

Presentation Title: ***Cyber Risks in an Ever-Changing Landscape***

Biographical Sketch: *Simona Rollinson is ISACA's Chief Operating Officer (COO), leading ISACA's technology team, driving the organization's continuing digital transformation, and exploring new opportunities for harnessing technology to elevate the educational and professional development experiences for ISACA's members and enterprise customers. She plays a key role in transforming ISACA's learning technology platform to support the professional community at all levels and stages, from individual development to enterprise solutions.*

Simona brings a wealth of technology leadership and strategy experience to ISACA, from her earlier roles as software engineer and developer, to president of Follett Software Company and later as CIO *for Cook County Government in Chicago, Illinois—a role for which she was named CIO of the Year. Most recently, she served as CIO for Clayco, a real estate development, architecture, engineering and construction firm. Throughout her executive career, Simona has led successful complex digital transformational change and evolution. The hallmarks of her recent tenure are establishing an enterprise architecture capability, modernizing many foundational systems and legacy platforms and a focus on improved vendor and project management. She holds ISACA's CISM, CRISC and CDPSE certifications.*

Tuesday Dinner Keynote: 7:00 PM Tuesday, March 1, 2022

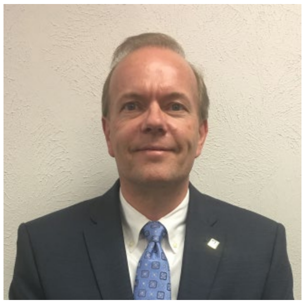


Fouad Teymour, *S.C. Johnson Professor of Chemical Engineering and Director of the Center for Complex Systems and Dynamics, Illinois Institute of Technology*

Presentation Title: ***Diversity, Perfect Mixing, Symmetry, and Autocatalysis: Random thoughts on celebrating differences.***

Biographical Sketch: *Fouad Teymour is Johnson Polymer Professor in the department of Chemical and Biological Engineering, and the Director of the Center for Complex Systems and Dynamics, at the Illinois Institute of Technology. He is a researcher and award-winning educator. His research focuses in the areas of polymer reaction engineering, nonlinear dynamics, complexity, biofuels, and drug delivery. He is also a Chicago-based Egyptian American playwright whose plays have been produced on Chicago theater stages (Silk Road Rising 2019, Three Cat Productions 2017).*

Wednesday Morning Keynote: 8:30 AM Wednesday, March 2, 2022



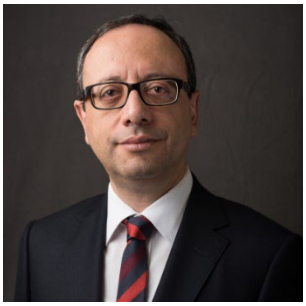
Henrik Rasmussen, *Vice President of Catalyst and Technology and Managing Director for the Americas, Haldor Topsoe*

Presentation Title: ***The Blue and Green Energy Translation***

Biographical Sketch: *Henrik Rasmussen graduated from the University of Copenhagen in 1989 with a degree in chemical engineering before relocating to the United States in 1991. He has worked at Haldor Topsoe for over 32 years and has held many technical and management positions for all Topsoe's business units. His technical expertise covers the Ammonia, MeOH and Hydrogen plant industry and specifically the refining industry for both catalyst and technology. In the last few years, Henrik has been heavily involved with Topsoe's green and blue process technologies for the production of renewable fuels, green and blue Ammonia, MeOH and hydrogen.*

Since 2007, Mr. Rasmussen has been the Vice President of Catalyst and Technology with responsibility of Topsoe's catalyst and license technology business for the U.S., Canada, and the Caribbean. In early 2021, Henrik assumed the role as Managing Director for the Americas responsible for Topsoe business in North and South America with offices in Houston, Los Angeles, Mexico, Brazil and Argentina.

Wednesday Afternoon Keynote: 1:00 PM Wednesday, March 2, 2022



Manos Mavrikakis, *Ernest Micek Distinguished Chair, James A. Dumesic Professor, and Vilas Distinguished Achievement Professor, University of Wisconsin-Madison*

Presentation Title: ***An atomic-scale perspective on catalyst's stability and on the nature of the active site when the reaction is taking place***

Biographical Sketch: *Manos Mavrikakis is the Ernest Micek Distinguished Chair, the James A. Dumesic Professor, and the Vilas Distinguished Achievement Professor of Chemical Engineering at the University of Wisconsin-Madison. He received a Diploma in Chemical Engineering from NTUA in Greece, and a PhD in Chemical Engineering & Scientific Computing from the University of Michigan, Ann Arbor. Following postdocs at the University of Delaware and the Technical University of Denmark, he joined the faculty of Chemical Engineering at UW-Madison in 1999. His main research interests include the elucidation of detailed reaction mechanisms for thermal heterogeneously catalyzed and electrocatalyzed reactions and the identification of improved catalytic materials from first-principles-based microkinetic modeling. Bridging the pressure gap between UHV experiments and atmospheric/higher pressure experiments in catalysis has been at the heart of his work.*

Mavrikakis has been elected Fellow of APS (2013), AAAS (2014), and AVS (2016). He served as his Department Chair (2015-2018) and was a Visiting Miller Research Professor at UC Berkeley – Chemistry in 2019. He received the 2009 Paul H. Emmett award from the North American Catalysis Society, the 2014 R. H. Wilhelm award from AIChE, the 2019 Gabor A. Somorjai award from ACS, and the 2021 Robert Burwell Lectureship from the North American Catalysis Society. He served as editor-in-chief of Surface Science between 2012 and 2020.

Session Presentations (Day 1)

Tuesday, March 1, 2022

Conference Welcome
Tuesday, March 1, 2022 (**TuI1**)
8:15 AM **Conference Introduction**
Matthew Walters (Conference Chair, Exponent)
Jessica Morris (Conference Co-Chair, Exponent)
8:25 AM **AIChE Chicago Introduction**
Ha Dinh (Local Section Chair, Honeywell UOP)

Tuesday Morning Keynote Session
Tuesday, March 1, 2022 (**TuK1**)
8:30 AM **Keynote Introduction**
Matthew Walters (Conference Chair, Exponent)
8:35 AM **Lessons Learned from the AB Specialty Silicones Explosion and Fire Incident**
Stephen Klejst & Vonzella Vincent (U.S. Chemical Safety and Hazard Investigation Board)

Process Safety I
Tuesday, March 1, 2022 (**TuA1**)
Chair: *Ashok Dastidar* (Fauske & Associates)
Co-chair: *Neal Muller* (Stepan Company)
9:40 AM **The Next Chapter in Global Compliance Auditing** (TuA1a)
Hope Luebeck (The Chemours Company)
10:00 AM **MOC 101 – Fundamentals for Effective Change Management** (TuA1b)
Nancy Fulk & Camila Costa da Fonseca (Siemens Energy)
10:20 AM **Learnings in Material Flash Point Characterization from the Lac-Mégantic Rail Disaster** (TuA1c)
Trevor Lardinois (Exponent)

Polymer Science
Tuesday, March 1, 2022 (**TuA2**)
Chair: *Karthika Suresh* (University of Illinois Chicago)
Co-Chair: *Carina Martinez* (University of Illinois Chicago)
9:40 AM **Effects of Additives on Properties of Chitosan Composite Films** (TuA2a)
Shu Xu (Argonne National Laboratory)
10:00 AM **Extensional Rheology and Pinching Dynamics of Polysaccharide Food Thickener** (TuA2b)
Karthika Suresh (University of Illinois at Chicago)
10:20 AM **Mapping the Spinnability of PEO Fibers Via Centrifugal Force Spinning Using Rheology and Evaporation** (TuA2c)
Cheryl Slykas (University of Illinois Chicago)

Process Safety II
Tuesday, March 1, 2022 (**TuB1**)
Chair: *Neal Muller* (Stepan Company)
Co-chair: *Ashok Dastidar* (Fauske & Associates)
11:10 AM **Towards Safer Practices in Academic and Industrial Chemical Laboratories** (TuB1a)
Sopuruchukwu Ezenwa (Purdue University)
11:30 AM **Mechanics of Hot Caustic Solution Eruptions** (TuB1b)
David Hietala (Exponent)
11:50 AM **The Long Road to a Unified Combustible Dust Standard – NFPA 660** (TuB1c)
Ashok Dastidar (Fauske & Associates)

Bioengineering & Nanotechnologies I
Tuesday, March 1, 2022 (**TuB2**)
Chair: *Wujie Zhang* (Milwaukee School of Engineering)
Co-chair: *Meltem Urgun-Demirtas* (Argonne National Laboratory)
11:10 AM **Biochemical Characterization and Applications of Upland Cress Biosynthesized Gold Nanoparticles** (TuB2a)
Noah Hutchinson (Milwaukee School of Engineering)
11:30 AM **Development of Nanosilicate-Hydrogel Composites for Sustained Delivery of Charged Biopharmaceutics** (TuB2b)
Samuel Stealey (Saint Louis University)
11:50 AM **Microfluidic Chips: Introduction, Production and Application in Chemical Engineering or Bioengineering** (TuB2c)
Sal Hussaini (University of Colorado Boulder)

Tuesday Afternoon Keynote Session

Tuesday, March 1, 2022 (**TuK2**)

12:45 PM **Keynote Introduction**
Jessica Morris (Exponent)

12:50 PM **Cyber Risks in an Ever-Changing Landscape**
Simona Rollinson (ISACA)

Environmental Compliance & Remediation I

Tuesday, March 1, 2022 (**TuC1**)
Chair: *Shri Dawande* (Honeywell UOP)
Co-Chairs: *Aditya Prajapati* (Lawrence Livermore National Laboratory), *Yechan Won* (Geosyntec Consultants)

2:00 PM **Electrochemical Treatment of Perfluoroalkyl Substances in Aqueous Film Forming Foams Using Reactive Electrochemical Membranes** (TuC1a)
Saurabh Misal (University of Illinois Chicago)

2:20 PM **Utilizing Capping Methods and Sorbent Amendments As a Remediation Strategy for Pfas-Contaminated Sediments** (TuC1b)
Hossein Dallalzadeh Atoufi (Illinois Institute of Technology)

2:40 PM **Pfas Electro-Exidation in Tubular Ti4O7 Membranes : Effect of Concentration and Background Matrix** (TuC1c)
Shirin Saffar Avval (University of Illinois Chicago)

3:00 PM **Investigation of the Use of Magnéli-Phase Titanium Oxide Membranes for Ex-Situ Electrochemical Treatment of Pfas-Contaminated Groundwater** (TuC1d)
Suzane Carneiro (University of Illinois Chicago)

Bioengineering & Nanotechnologies II

Tuesday, March 1, 2022 (**TuC2**)
Chair: *Wujie Zhang* (Milwaukee School of Engineering)
Co-chair: *Meltem Urgun-Demirtas* (Argonne National Laboratory)

2:00 PM **Design of Novel Bioink Containing Gelatin-Coated Microspheres for Bioprinting** (TuC2a)
Muskan Kanungo (Milwaukee School of Engineering)

2:20 PM **Biocompatible Peg Diacrylate Hydrogel Nanocomposite Emulsion Scale Down for siRNA Drug Delivery Platforms** (TuC2b)
Ruth Negru (Illinois Institute of Technology)

2:40 PM **Controlled Release of Cytokines By Biodegradable Toroidal Spiral Particles for Enhancement of Localized CAR-T Cell Therapy** (TuC2c)
Abigail Hartzell (University of Illinois Chicago)

3:00 PM **Development of the Cellmag-Carwash System for Isolation of Pure Single Cell Populations** (TuC2d)
Brittany Rupp (University of Michigan)

Environmental Compliance & Remediation II

Tuesday, March 1, 2022 (**TuD1**)
Chair: *Aditya Prajapati* (Lawrence Livermore National Laboratory)
Co-Chairs: *Shri Dawande* (Honeywell UOP)**,** *Yechan Won* (Geosyntec Consultants)

3:30 PM **A Membrane-Based Desalination Technology for Reuse and Recovery of Produced Water** (TuD1a)
Hossein Dallalzadeh Atoufi (Illinois Institute of Technology)

3:50 PM **Simulation of Pollutants Distribution for an Impulse Input in Free Streams** (TuD1b)
Seyed Javad Amirfakhri (University of Wisconsin – Stevens Point)

4:10 PM **Defluoridation of Water Using Aluminum Coated Sand Sorbent** (TuD1c)
Kiana Modaresahmadi (University of Illinois Chicago)

4:30 PM **Design of an Electric Field-Assisted Water-Gradient System for CO2 Capture** (TuD1d)
Rohan Sartape (University of Illinois Chicago)

Machine Learning & Optimization

Tuesday, March 1, 2022 (**TuD2**)
Chair: *Noah Paulson* (Argonne National Laboratory)
Co-chair: *Hakim Iddir* (Argonne National Laboratory)

3:30 PM **Machine Learning for Large Scale Dynamic Systems Based on Model Reduction Technique and Orthogonal Experimental Design Method** (TuD2a)
Weiguo Xie (University of Minnesota Duluth)

3:50 PM **An Efficient Reinforcement Algorithm Approach to Stochastic Optimal Control with Application to Biodiesel Production** (TuD2b)
Shiam Kannan (Vishwamitra Research Institute)

4:10 PM **Accelerated Discovery of Energy Storage Materials Via Multiobjective Bayesian Optimization** (TuD2c)
Hieu Doan (Argonne National Laboratory)

4:30 PM **Generalized Global Sustainability Model (GGSM) to Study Food-Energy-Water (FEW) Nexus** (TuD2d)
Apoorva Nisal (University of Illinois Chicago)

Poster Session

Tuesday, March 1, 2022 (**TuP1**)
Chair: *Karthika Suresh* (University of Illinois Chicago)
Co-chair: *Daniel Christiansen* (University of Illinois Chicago)
5:00 PM Poster Session

Poster 1 **WITHDRAWN** (TuP1c)

Poster 2 **Understanding the Mechanisms and Feasibility of Solar-Radiation-Enhanced Ammonia Synthesis** (TuP1d)
Carissa Yim (University of Michigan)

Poster 3 **An Evaluation Method for Energy Performance of Sulfur Recovery Units and Tail Gas Treatment Units Based on Grey Correlation Analysis** (TuP1f)
Min Qiu (China University of Petroleum, Beijing)

Poster 4 **Experimental Investigation on the Gas–Liquid Separation Performance of Vane Separators with Bio-Inspired Functional Surfaces** (TuP1g)
Jiarong Wang (China University of Petroleum, Beijing)

Poster 5 **Computational Study of on-Surface and Sub-Surface Oxygen in Rh(111)** (TuP1h)
Weronika Walkosz (Lake Forest College)

Poster 6 **Impact of Anion Species in the Biosorption of Nickel and Lead By *Lemna m*.** (TuP1h)
Magdalene Jones (University of Minnesota Duluth)

Poster 7 **Machine Learning Prediction of Hydration and Ion Association Properties of Zwitterions** (TuP1h)
Daniel Christiansen (University of Illinois Chicago)

Local Section Dinner and Dinner Keynote

Tuesday, March 1, 2022 (**TuK3**) [**Zoom signup link**]

6:30 PM **Networking**

6:45 PM **Local Section Announcements**
Ha Dinh (Honeywell UOP)

6:55 PM **Keynote Introduction**
Hadjira Iddir (Becht)

7:00 PM **Diversity, Perfect Mixing, Symmetry, and Autocatalysis: Random thoughts on celebrating differences.**
Fouad Teymour (Illinois Institute of Technology)

Session Presentations (Day 2)

Wednesday, March 2, 2022

Conference Welcome

Wednesday, March 2, 2022 (**WeI1**)

8:25 AM **Conference Introduction**
Matthew Walters (Conference Chair, Exponent)

Wednesday Morning Keynote Session

Wednesday, March 2, 2022 (**WeK1**)

8:30 AM **Keynote Introduction**
Belma Demirel (bp)

8:35 AM **The Blue and Green Energy Translation**
Henrik Rasmussen (Haldor Topsoe)

Refining & Renewables

Wednesday, March 2, 2022 (**WeA1**)
Chair: *Belma Demirel* (bp)
Co-Chairs: *Hadjira Iddir* (Becht), *Meltem Urgun-Demirtas* (Argonne National Laboratory)

9:40 AM **Why and How Refineries Will Drive the Transition from Fossil to Renewable Fuels** (WeA1a)
Peter Nymenn (Haldor Topsoe)

10:00 AM **Unlocking the Potential of Existing Hydrotreaters for Processing Renewable Feedstocks** (WeA1b)
Aline Bueno (Albemarle)

10:20 AM **Life Cycle Greenhouse Gas Implications of Blending Performance-Enhancing Bioblendstocks at Refineries: Integrated Refinery Optimization and Life Cycle Analysis** (WeA1c)
Troy Hawkins (Argonne National Laboratory)

10:40 AM **Life Cycle Analysis of Plastic to Fuel and Plastic Circular Economy** (WeA1d)
Ulises R. Gracida-Alvarez (Argonne National Laboratory)

Climate Solution: Action I

Wednesday, March 2, 2022 (**WeA2**)
Chair: *Dennis O'Brien* (Advisian)

9:40 AM **Greenhouse Gas Emissions at the Metropolitan Water Reclamation District of Greater Chicago** (WeA2a)
Joseph Kozak & Jonathan Grabowy (Metropolitan Water Reclamation District of Greater Chicago)

10:00 AM **Improved Bio-chemical Utilization of Indoor, Aquaponic Growing Systems** (WeA2b)
Blake Davis (Illinois Institute of Technology)

10:20 AM **The Changing Energy Storage Landscape** (WeA2c)
George Crabtree (University of Illinois Chicago/ Argonne National Laboratory)

Catalysis & Reaction Engineering I

Wednesday, March 2, 2022 (**WeB1**)
Chair: *Trevor Lardinois* (Exponent)
Co-Chair: *Belma Demirel* (bp)

11:10 AM **Catalytic Hydrogenolysis of Polyolefin Waste to Higher Value Liquid Products** (WeB1a)
Ryan Hackler (Argonne National Laboratory)

11:30 AM **Non-Oxidative Dehydroaromatization of Long-Chain Alkanes on Intermetallic Surface** (WeB1b)
Ranjan Behera (Iowa State University)

11:50 AM **Assessment of Catalysts for Oxidative Coupling of Methane and Ethylene** (WeB1c)
Jordy Ramos-Yataco (Northwestern University)

Climate Solution: Action II

Wednesday, March 2, 2022 (**WeB2**)
Chair: *Dennis O'Brien* (Advisian)

11:10 AM **Material Flow Analysis of Polyurethane** (WeB2a)
Chao "Chloe" Liang (Northwestern)

11:30 AM **Nuclear Energy and Energy Sustainability: Resources, Environment and Climate** (WeB2b)
Pavel Tsvetkov (Texas A&M)

11:50 AM **WITHDRAWN** (WeB2c)

Wednesday Afternoon Keynote Session

Wednesday, March 2, 2022 (**WeK2**)

1:00 PM **Keynote Introduction**
Hakim Iddir (Argonne National Laboratory)

1:05 PM **An atomic-scale perspective on catalyst's stability and on the nature of the active site when the reaction is taking place**
Manos Mavrikakis (University of Wisconsin-Madison)

Catalysis & Reaction Engineering II

Wednesday, March 2, 2022 (**WeC1**)
Chair: *Trevor Lardinois* (Exponent)
Co-Chair: *Belma Demirel* (bp)

2:10 PM **Highly Selective Atomically Dispersed Copper Electrocatalyst for CO2 Reduction to Ethanol** (WeC1a)
Haiping Xu (Argonne National Laboratory)

2:30 PM **Bimetallic Ru-Based Alloy Nanoparticles: Unravelling the Effects of in Addition on Methanol Synthesis from CO2** (WeC1b)
Feiyang Geng (University of Notre Dame)

2:50 PM **First-Principles Analysis of the Ammonia Decomposition Reaction on High Entropy Alloy Catalysts** (WeC1c)
Zuhal Cakir (Purdue University)

3:10 PM **WITHDRAWN** (WeC1d)

Energy Storage I

Wednesday, March 2, 2022 (**WeC2**)
Chair: *Hakim Iddir* (Argonne National Laboratory)
Co-Chair: *Juan Garcia* (Argonne National Laboratory)

2:10 PM **A Unique Co-Free Cathode for High Energy Li-Ion Cells** (WeC2a)
Boyu Shi (Argonne National Laboratory)

2:30 PM **Insights from Computational Studies on the Anisotropic Volume Change of LixNiO2 at High State of Charge (x < 0.25)** (WeC2b)
Juan Garcia (Argonne National Laboratory)

2:50 PM **Probing the Impedance at Low States of Charge in Li- and Mn-Rich Oxides** (WeC2c)
Arturo Gutierrez (Argonne National Laboratory)

3:10 PM **Electrolyte Engineering to Stabilize Cathode-Electrolyte Interface of Na1-XFeO2 Cathode for Na-Ion Batteries** (WeC2d)
Jehee Park (Argonne National Laboratory)

Fluid Properties, Fluid Dynamics, & Transport Phenomena

Wednesday, March 2, 2022 (**WeD1**)
Chair: *Robert Tsai* (Honeywell UOP)
Co-Chair: *Karthika Suresh* (University of Illinois Chicago)

3:40 PM **Development on Measurement Technology for Studying Mixing and Reaction State Using Online Electrical Resistance Tomography** (WeD1a)
Weiguo Xie (University of Minnesota Duluth)

4:00 PM **Using Molecular Dynamics to Study Separation Mechanisms of Monoatomic Gases Via DD3R Zeolite Membrane** (WeD1b)
Bandar Bashmmakh (Illinois Institute of Technology)

4:20 PM **Foam Film Drainage of Milk Protein Derivative Nacas Vs Micellar Surfactant SDS** (WeD1c)
Lena Hassan (University of Illinois Chicago)

4:40 PM **Rheology and Texture of Animal and Plant-Based Mayo Emulsions** (WeD1d)
Nadia Nikolova (University of Illinois Chicago)

Energy Storage II

Wednesday, March 2, 2022 (**WeD2**)
Chair: *Juan Garcia* (Argonne National Laboratory)
Co-Chair: *Hakim Iddir* (Argonne National Laboratory)

3:40 PM **V2+/V3+ Reaction Intermediate By Surface Enhanced Raman Spectroscopy** (WeD2a)
Daniel Pert (University of Michigan)

4:00 PM **Compressed Gas Energy Storage Integrated with Combined Heat and Power Plant** (WeD2b)
Sebastiano Giardinella (University of Illinois Urbana-Champaign)

4:20 PM **Active Learning for the Design of Naturally Occurring Organic Redox-Active Materials for Non-Aqueous Redox Flow Batteries** (WeD2c)
Akash Jain (Argonne National Laboratory)

4:40 PM **Development of Eco-Friendly Phase Change Material for Low Temperature Energy Storage Applications** (WeD2d)
Kamal Nayan (Rajiv Gandhi Institute of Petroleum Technology)

Presentation Abstracts (Day 1)

Tuesday, March 1, 2022

<u>**Tuesday Morning Keynote Session**</u>
Tuesday, March 1, 2022 (**WeK1**)

8:35 AM Lessons Learned from the AB Specialty Silicones Explosion and Fire Incident (TuA1a)

Stephen Klejst (CSB), *Vonzella Vincent* (CSB)

The presentation will focus on the explosion and fire incident that occurred at the AB Specialty Silicones facility on May 3, 2019 in Waukegan, Illinois.

The incident occurred while performing a batch operation that involved manually adding and mixing chemicals in a tank inside the production building. During the operation, an operator pumped an incorrect chemical into the tank, which was incompatible with another chemical that was added to the tank. After the incompatible chemicals were mixed, the tank contents underwent a chemical reaction causing a process upset in which the tank contents foamed and overflowed from the tank's top opening. During the process upset, hydrogen gas was produced and ignited causing a massive explosion and fire. The explosion fatally injured four employees and caused significant property damage.

The presentation will include the cause of the incident and a discussion of the significant safety issues identified during CSB's investigation:

- Mixing of Incompatible Materials
- Effectiveness of the ABSS Hazard Analysis Program
- Storage and Handling of Incompatible Materials
- Batch Equipment and Ventilation System Design
- Gas Detection and Alarm System
- Double Initial Procedure Program
- Process Safety Culture
- Safety Management System that Addresses Process Safety

<u>**Process Safety I**</u>
Tuesday, March 1, 2022 (<u>**TuA1**</u>)
Chair: *Ashok Dastidar* (Fauske & Associates)
Co-chair: *Neal Muller* (Stepan Company)

9:40 AM The Next Chapter in Global Compliance Auditing (TuA1a)

Hope Luebeck (The Chemours Company)

The recent pandemic spurred evolutionary changes to how risk management programs are executed across the globe. Compliance verifications had to continue despite the inability of audit teams to visit sites for a first-hand evaluation of program status. Audit teams were driven to innovate to accomplish their mission. This metamorphosis has forever changed the process by which compliance auditing is conducted.

This presentation will discuss features such as planning tips, audit strategies, auditor utilization, and various tools that audit teams can employ and how these aspects will affect the future of post-pandemic compliance auditing.

10:00 AM AM MOC 101 – Fundamentals for Effective Change Management (TuA1b)

Nancy Fulk (Siemens Energy), *Camila Costa da Fonseca* (Siemens Energy)

Management of Change (MOC) is the cornerstone of a successful risk-based process safety (RBPS) program. Safe operation and maintenance of facilities that manufacture or store hazardous chemicals require robust process safety management systems. The MOC element of an RBPS establishes a formal, documented, and authorization process for any proposed changes, to manage changes which may introduce unexpected new hazards or increase the risk of existing hazards. Furthermore, the MOC process ensures that changes are communicated to potentially affected personnel, as well as ensures that all affected documentation is updated.

A poor MOC program has been a root cause in several process safety incidents, including the Flixborough disaster. The temporary modifications did not go through a proper review process; an effective MOC program could have discovered the design flaws before the change was implemented and prevented the explosion. In addition to case studies such as this, this paper will provide an overview of best management practices and essential features for the MOC element, which can be used as a basis to develop or evaluate existing MOC management systems, and as a result play a role in identifying hazards, managing risk, and sustaining safe operations.

10:20 AM Learnings in Material Flash Point Characterization from the Lac-Mégantic Rail Disaster (TuA1c)

Trevor Lardinois (Exponent), *David Hietala* (Exponent), *Brenton Cox* (Exponent), *Sean Dee* (Exponent), *Russell Ogle* (Exponent), *Matt Walters* (Exponent)

The flash point of ignitable liquids influences the product hazard classification, as well as the requirements for safe handling, storage, and shipping. However, flash point determination is less straightforward for complex multi-component mixtures or non-homogenously dispersed liquid emulsions. Here, we address the complexity of compositional changes and their impact on material flammability as a function of time and lot-to-lot variation. The flash point of Bakken crude, which was involved in the Lac-Mégantic Rail Disaster in 2013, serves as a case study of such phenomenon, with significant variability in material flash point. The observed variation in the flash point of Bakken crude stems from the off-gassing of more volatile, lower-molecular weight hydrocarbons, increasing the flash point as a function of time. Additionally, the site-specific collection of Bakken crude results in variations in composition make-up and, therefore, introduces variability in flash point. Lessons learned from the Lac-Mégantic Rail Disaster will be discussed to emphasize the importance of a thorough understanding of material flammability properties, including how these properties can potentially change during handling, storage, and shipping.

<u>Polymer Science</u>

Tuesday, March 1, 2022 (<u>**TuA2**</u>)
Chair: *Karthika Suresh* (University of Illinois Chicago)
Co-chair: *Carina Martinez* (University of Illinois Chicago)

9:40 AM Effects of Additives on Properties of Chitosan Composite Films (TuA2a)

Shu Xu (Argonne National Laboratory), *Sean Riggio* (Argonne National Laboratory), *Meltem Urgun-Demirtas* (Argonne National Laboratory)

The accumulation of plastic waste in the environment continues to be a growing concern worldwide. There is an increasing interest for production of alternative materials for single-use plastics, but production of the sustainable packaging materials is still at prefatory stage. Chitosan is a semi-crystalline carbohydrate polymer obtained via the deacetylation of chitin, an oligosaccharide found in the shells of crabs and shellfish. Chitosan has been the subject of large amounts of research due its film-forming ability, biodegradability, and solubility. Chitosan also possesses antimicrobial properties, which makes it an ideal material in food packaging applications. Chitosan films tend to have excellent mechanical strength, but generally require modification via the addition of other polymers or plasticizers to counteract their inherent brittleness. Common plasticizers such as glycerol and addition of other film-forming polymers such as starch have been shown to increase percent elongation relative to chitosan films. However, the water vapor transmission rate of plasticized chitosan films also increases concomitantly. This study aims to investigate the change of physicochemical properties of polymer films, including the mechanical and water vapor permeation properties, with additives such as commercially available bananas, potatoes, and table sugar. This presentation will also cover the effect of these additives on the biodegradability of chitosan films.

10:00 AM Extensional Rheology and Pinching Dynamics of Polysaccharide Food Thickener (TuA2b)

Karthika Suresh (University of Illinois Chicago), *Michael Boehm* (Motif FoodWorks), *Stefan Baier* (Motif Foodworks), *Vivek Sharma* (University of Illinois Chicago)

Foods are multicomponent soft materials that often contain dispersed drops, bubbles, particles, or proteins. Often protein-based foams, emulsions, suspensions, and pastes contain polysaccharides that act as binders, thickeners, gelling agents or rheology modifiers, and influence shelf-life, rheology, processability as well as control over texture, and mouth-feel. Stream-wise velocity gradients associated with extensional flows spontaneously arise during extrusion, dispensing, bubble growth or collapse as well as consumption including swallowing and suction via straws. Even though shear rheology response is fairly well characterized and utilized in food industry, elucidating, measuring and harnessing the extensional rheology response have remained longstanding challenges. The characterization challenges include the lack of robust, reliable and affordable methods for measuring extensional rheology response, whereas the product design challenges stem from the difficulties in assessing or predicting the influence of macromolecular properties on macroscopic rheological behavior. In this contribution, we address the characterization challenges for specific case of xanthan gum thickener by using dripping-onto-substrate (DoS) rheometry protocols that we developed that rely on analysis of capillary-driven thinning and break-up of liquid necks created by releasing a finite volume of fluid onto a substrate. The DoS rheometry protocols emulate the heuristic tests of thickening, stickiness or cohesiveness based on dripping a sauce from a ladle or dispensing from a nozzle onto a substrate. We investigate the concentration-dependent variation in shear and extensional rheology of xanthan gum solutions. We show that changing salt concentration can be used for tuning the pinch-off dynamics, extensional rheology response, and processability of xanthan gum solutions.

10:20 AM Mapping the Spinnability of PEO Fibers Via Centrifugal Force Spinning Using Rheology and Evaporation (TuA2c)

Cheryl Slykas (University of Illinois Chicago), *Jorgo Merchiers* (University of Hasselt), *Carina Martinez* (University of Illinois Chicago), *Naveen Reddy* (University of Hasselt), *Vivek Sharma* (University of Illinois Chicago)

In this contribution, we explore how poly(ethylene oxide) (PEO) fiber spinnability via centrifugal force spinning is affected by solvent choice by using different mixtures of acetonitrile and water ratios. We determined that the spinnability and fiber morphology depend on solvent choice when polymer concentration, solution shear and extensional rheology, number of entanglements, and processing conditions are nearly matched.

Process Safety II

Tuesday, March 1, 2022 (**TuB1**)
Chair: *Neal Muller* (Stepan Company)
Co-chair: *Ashok Dastidar* (Fauske & Associates)

11:10 AM Towards Safer Practices in Academic and Industrial Chemical Laboratories (TuB1a)

Sopuruchukwu Ezenwa (Purdue University), *Abhijit Talpade* (Purdue University), *Pushkar Ghanekar* (Purdue University), *Jeremy Arvay* (Purdue University), *Ravi Joshi* (Purdue University), *Samuel Kravitz* (Purdue University), *Vikrant Gajria* (Purdue University), *Anirudh Tunga* (Purdue University), *Jayachandran Devaraj* (Corteva Agriscience), *Fabio H. Ribeiro* (Purdue University), *Ray A. Mentzer* (Purdue University)

The U.S. Chemical Safety Board (CSB) has noted that safety incidents are prevalent in laboratory settings at academic, industrial, and government research facilities. These trends suggest a need for broad and systematic changes in safety practices that go beyond mere compliance to established safety standards. To this end, our safety team composed of members from two multi-institution research centers (Purdue Process Safety and Assurance Center (P2SAC) and Center for Innovative and Strategic Transformation of Alkane Resources (CISTAR)) is investigating ways to improve safety practices in laboratories. We surveyed current safety practices at chemical laboratories within our academic and industrial partners. Key areas of improvement and recommended best practices were established. Furthermore, we identified the need for a convenient web tool that conducts preliminary hazard analyses. To address this, we developed Reactive Hazards Evaluation Analysis and Compilation Tool (RHEACT) that extracts information from user-supplied operation parameters and from parsed safety data sheets (SDS). This tool further generates an operational hazard matrix, calculates adiabatic temperature rise, and generates a chemical compatibility matrix, all of which provides a user with a broad initial evaluation of potential hazards. Taken together, these safety initiatives will contribute to promoting safer practices and reducing the occurrence of safety incidents in chemical labs.

11:30 AM Mechanics of Hot Caustic Solution Eruptions (TuB1b)

David Hietala (Exponent), *Brenton Cox* (Exponent), *Russell Ogle* (Exponent), *Matt Walters* (Exponent)

Sodium hydroxide is an extremely versatile chemical that can be found in many commercial drain cleaners, among many other applications. However, sodium hydroxide is also a hazardous chemical and must be carefully handled. In addition to being a corrosive chemical, it exhibits an exothermic heat of dilution when mixed in water. The safe procedure for making a caustic solution is to mix solid sodium hydroxide gradually into cold water while stirring the mixture. The alternative, unsafe, procedure is to quickly add sodium hydroxide into hot water without stirring. The unsafe procedure can create a boiling solution and, under the right conditions, cause an eruption of hot caustic solution from its container. In this investigation we present a simplified analysis of the eruption mechanics to demonstrate the magnitude of the hazard. We establish a maximum threshold temperature of the receiving water that should not be crossed and describe the influence of the container shape on the potential for eruption.

11:50 AM The Long Road to a Unified Combustible Dust Standard – NFPA 660 (TuB1c)

Ashok Dastidar (Fauske & Associates)

Dust explosions are a serious hazard in the process industries that can lead to the loss of life as well as destruction of property. Currently there is no government regulation protecting workers from this hazard except in the grain handling field. However, there are been a group of consensus standards by the National Fire Protection Association that have been incorporated into fire and building standards. These myriad of industrial occupancy standards have a long history and have helped mitigate and protect against combustible dust fires and explosions. Unfortunately, the large number of standards and their overlapping applicability have led to confusion for the end user and code enforcers. This presentation will provide a brief overview on the history of dust explosion and the path to developing one comprehensive combustible dust standard.

Bioengineering & Nanotechnologies I

Tuesday, March 1, 2022 (**TuB2**)
Chair: *Wujie Zhang* (Milwaukee School of Engineering)
Co-chair: *Meltem Urgun-Demirtas* (Argonne National Laboratory)

11:10 AM Biochemical Characterization and Applications of Upland Cress Biosynthesized Gold Nanoparticles (TuB2a)

Noah Hutchinson (Milwaukee School of Engineering), *Muskan Kanungo* (Milwaukee School of Engineering), *Wujie Zhang* (Milwaukee School of Engineering)

This research focuses on the plant-mediated biosynthesis process for the production of gold nanoparticles (Au NPs) using upland cress (Barbarea verna), as various biomolecules within the upland cress act as both reducing and capping agents. The biosynthesized gold nanoparticles were thoroughly characterized using UV-vis spectroscopy, surface charge (zeta potential) analysis, scanning electron microscopy-energy-dispersive X-ray spectroscopy (SEM-EDX), atomic force microscopy (AFM), and X-ray diffraction (XRD). The results indicated the synthesized Au NPs are spherical and well-dispersed with an average diameter around 12-15 nm and a characteristic absorbance peak at ~ 529 nm. EDX results showed a 11.13% gold content. Colloidal Au NP stability was confirmed with a zeta potential (ζ) value of -36.8 mV. X-ray diffraction analysis verified the production of crystalline face-centered cubic gold. Moreover, the antimicrobial activity of the Au NPs was evaluated using Gram-negative E. coli and gram-positive Bacillus megaterium. Results demonstrated concentration-dependent antimicrobial properties. Lastly, applications of the Au NPs in catalysis and biomedicine were evaluated. The catalytic activity of Au NPs was demonstrated through the conversion of 4-nitrophenol to 4-aminophenol which followed first-order kinetics. Cellular uptake and cytotoxicity were evaluated using both BMSCs (stem) and HeLa (cancer) cells and the results were cell type dependent. The biosynthesized Au NPs show great potential for various applications such as catalysis, pharmaceutics, and biomedicine.

11:30 AM Development of Nanosilicate-Hydrogel Composites for Sustained Delivery of Charged Biopharmaceutics (TuB2b)

Samuel Stealey (Saint Louis University)

Nanocomposite hydrogels containing two-dimensional nanosilicates (NS) have emerged as a new technology for prolonged delivery of biopharmaceuticals. However, little is known about the physical-chemical properties governing the interaction between NS and proteins and the release profiles of NS-protein complexes in comparison to traditional poly(ethylene glycol) (PEG) hydrogel technologies. To fill this gap in knowledge, we fabricated a novel nanocomposite hydrogel composed of PEG and Laponite and identified simple but effective experimental conditions to obtain sustained protein release, up to 23 times slower as compared to traditional PEG hydrogels, as determined by bulk release experiments and fluorescence correlation spectroscopy. Slowed protein release was attributed to the formation of NS-protein complexes, as NS-protein complex size was inversely correlated with protein diffusivity and release rates. While protein electrostatics, protein concentration and incubation time were important variables to control protein-NS complex formation, we found that one of the most significant and thus far less appreciated variable to obtain sustained release of bioactive proteins was the buffer chosen for preparing the initial suspension of the NS particles. The buffer was found to control the size of the nanoparticles, the absorption potential, the morphology, and stiffness of the hydrogels. From these studies, we conclude that the novel PEG-Laponite composite fabricated is a promising new platform for sustained delivery of positively charged protein therapeutics.

11:50 AM Microfluidic Chips: Introduction, Production and Application in Chemical Engineering or Bioengineering (TuB2c)

Sal Hussaini (University of Colorado Boulder)

To investigate the behavior of fluid in a controlled way with a transport regime of 10-9 to 10-4 m, microfluidic devices or systems have been used. It has advantageous features of high analysis speed, low sample volume, improved efficiency and functioning by adding different components in individual devices or systems known as micro total analysis systems (µTAS)/lab on a chip (LOC). The microphase enhances the surface area to volume ratio of systems (or devices) that ultimately improves the heat and mass transfer rate. The best example of systems which are multiphase in nature are biological where fluid are multiphase in nature and flows in human airways, cellular systems, flow in monoliths, interfacial forces appearing in microdevices (microfluidic devices). This microdevice helpful in the biological systems includes DNA analysis, cell encapsulation, cell stimulus and lysis.

Tuesday Afternoon Keynote Session

Tuesday, March 1, 2022 (**TuK2**)

12:50 PM Cyber Risks in an Ever-Changing Landscape

Simona Rollinson (ISACA)

IT risks loom larger than ever, especially amidst a global pandemic. High-profile cyberattacks are alarmingly frequent and affect organizations of every size and in every sector. Enterprises must worry about cyber risks – including ransomware attacks, malware intrusions, software and supply chain problems – as well as concerns brought by rapidly evolving technologies. Competing technology risks can make prioritizing difficult. Simona Rollinson, COO of ISACA and past Cook County CIO, will discuss cyber implications for adopting tech like the Internet of Things, cloud and artificial intelligence, as well as the future of cyber risk. Learn the steps you can take to ensure your enterprise is prepared, the questions you should ask to ensure proper oversight and governance, and what practices you can adopt to manage current cyber risk and challenges ahead.

Environmental Compliance & Remediation I

Tuesday, March 1, 2022 (**TuC1**)
Chair: *Shri Dawande* (Honeywell UOP)
Co-Chair: *Aditya Prajapati* (Lawrence Livermore National Laboratory)

2:00 PM Electrochemical Treatment of Perfluoroalkyl Substances in Aqueous Film Forming Foams Using Reactive Electrochemical Membranes (TuC1a)

Saurabh Misal (University of Illinois Chicago), *Danielle Tran* (CDM Smith), *Marzieh Shojaei* (Texas Tech University), *Isreq Real* (Texas Tech University), *Jennifer Guelfo* (Texas Tech University), *Charles Schaefer* (CDM Smith), *Brian Chaplin* (University of Illinois Chicago)

Electrochemical oxidation of per- and polyfluoroalkyl substances (PFAS) from a diluted aqueous film forming foam (AFFF) solution was performed using a tubular Ti4O7 reactive electrochemical membrane (REM). At a flux of 610 L m-2 h-1 and 40 mA cm-2 current density, results showed removal of long chained (C7 to C9) PFAS, such as perfluorinated carboxylates and perfluorinated sulfonates. Most of the short chained (C4 to C6) PFAS were formed until 4 h from the electrochemical oxidation of long chained PFAS, and showed removal after 4 h. The suspect analyses data primarily showed removal of polyfluorinated precursors and the formation of perfluorosulfonamides. The N-methyl perfluoroalkyl sulfonamido acetic acid compounds that were present or formed during the oxidation of the precursors, showed removal after 4 h. A combination of hydroxyl radical and direct electron transfer reactions was responsible for degradation of PFAS. Ion analysis showed formation of fluoride and sulfate ions for up to 2 h of electrolysis. Fluoride concentration at 2 h accounted for 84% of the total fluoride in the AFFF solution. The missing fluoride was attributed to formation of short chained PFAS and the decrease in fluoride concentration after 2 h was attributed to adsorption of fluoride on the REM. The energy consumption required for 90% defluorination was 27.3 W h L-1. The ability to electrochemically remove PFAS at low energy consumption indicates the REM is a promising technology for PFAS treatment.

2:20 PM Utilizing Capping Methods and Sorbent Amendments As a Remediation Strategy for Pfas-Contaminated Sediments (TuC1b)

Hossein Dallalzadeh Atoufi (Illinois Institute of Technology), *Prashik Manwatkar* (Illinois Institute of Technology), *David Lampert* (Illinois Institute of Technology)

Per- and polyfuoroalkyl substances (PFAS) are causing health and environmental problems in communities across the United States. Manufacturing and use of PFAS have been prevalent in the United States and worldwide since the 1940s. Surface water, groundwater, soil, and air can contain PFAS, regardless of where they originate, from remote rural to densely populated urban areas. Sediments are crucial components of aquatic environments that play a vital role in the health of organisms and ecosystems. The presence of PFAS in sediments is reported to be associated with other classes of anthropogenic pollutants. Aqueous film-forming foams, which are heavily used at airports and military bases, are a primary source of PFAS release in the environment. PFAS can also come from industrial and municipal discharges, wastewater treatment plants, agricultural runoff, and accidental spills. It, therefore, becomes essential to develop cost-effective in-situ remediation methods to mitigate the risks associated with contaminated sediments. This laboratory-scale research was designed as a replica of a field site contaminated with PFAS to examine the effectiveness of sediment caps for PFAS containment. This capping method was combined with sorbent materials to increase the performance of the system. Liquid chromatography with tandem mass spectrometry (LC/MS) is used to analyze samples for three of the most significant PFAS, including PFOA, PFOS, and PFBS. In the long term, this study seeks to understand PFAS fate and transportation and to develop a technology to prevent their mobilization and accumulation by capping them with a sorbent.

2:40 PM Pfas Electro-Exidation in Tubular Ti4O7 Membranes : Effect of Concentration and Background Matrix (TuC1c)

Shirin Saffar Avval (University of Illinois Chicago), *Mahsa Modiri Gharehveran* (Purdue University), *Linda Lee* (Purdue University), *Brian Chaplin* (University of Illinois Chicago)

Per- and polyfluoroalkyl substances (PFAS) has become a major concern in recent years. Recent studies have shown that PFAS could cause serious health effects. As a result, the EPA has set a health advisory level for Perfluorooctanoic acid (PFOA) and Perfluorooctanesulfonic acid (PFOS) at 70 parts per trillion. Their extensive use combined by their stability has caused the treatment of PFAS to be a difficult and expensive process. Here, we have studied PFAS electrochemical oxidation using TiO7 tubular membranes. Synthetic PFAS solutions were treated in a Ti4O7 reactive electrochemical membrane (REM) as a function of current density (30 to 40 mA/cm2) and PFAS concentration (0.1 to 10 µM). Results indicated that PFAS concentrations decreased by 96%- 99 % in 80 seconds of electrolysis time. Short chained intermediates were observed in these experiments and indicates sequential removal of CF2 groups. The total PFAS oxidation obeyed second-order kinetics, with rate constants of 4.9x106, 1.5x105, 2.7x104 M-1 s-1 for initial PFOA concentrations of 0.1, 1.4, and 10 µM, respectively. These results suggest that a preconcentration step might be beneficial for PFAS oxidation. To further understand the oxidation of short-chained PFAS, Perfluorobutanesulfonic acid (PFBS) was oxidized at 30 mA/cm2. The removal of PFBS was ~ 48% after 82 seconds of electrolysis times compared to 20% for the open circuit potential control experiment.

3:00 PM Investigation of the Use of Magnéli-Phase Titanium Oxide Membranes for Ex-Situ Electrochemical Treatment of Pfas-Contaminated Groundwater (TuC1d)

Suzane Carneiro (University of Illinois Chicago), *Mahsa Modiri Gharehveran* (Purdue University), *Linda Lee* (Purdue University), *Brian Chaplin* (University of Illinois Chicago)

Per- and polyfluoroalkyl substances (PFAS) are very stable synthetic chemicals widely used in daily applications such as in firefighting foams, cookware, and food packaging. These compounds cannot be destroyed using traditional biological or oxidative water treatment and tend to bioaccumulate, resulting in both environmental and health risks; therefore, the U.S. Environmental Protection Agency has issued a health advisory level of 70 parts per trillion (ppt) for the combined concentrations of the two most prevalent chemicals in the PFAS family, PFOA (perfluorooctanoic acid) and PFOS (perfluorooctanesulfonic acid). Electrochemical advanced oxidation processes are a promising ex situ remediation technology, where anodic polarization of a reactive electrochemical membrane (REM) results in degradation of PFAS through a combination of direct electron transfer reactions and reactions with hydroxyl radicals generated from water electrolysis. This work investigated the removal of PFAS from contaminated groundwater utilizing Magnéli-phase titanium oxide tubular reactive REMs. The groundwater used was from contaminated sites where aqueous film forming foams containing PFAS were used to suppress fires. The experiments were performed in full recycle, maintaning an elevated crossflow to prevent accumulation of oxygen bubbles on the electrode surface. Control experiments using synthetic groundwater spiked with PFAS indicated that higher permeate flow rates through the membrane results in higher PFOS removal. Synthetic groundwater oxidation at a constant current (37 mA/cm2) for 5 hours achieved 98%, and 93% removal of PFOS and PFOA, respectively, and the electrochemical treatment of groundwater resulted in removal of PFOS to below detection limit (< 0.4 nM) within 6 hours.

Bioengineering & Nanotechnologies II

Tuesday, March 1, 2022 (**TuC2**)
Chair: *Wujie Zhang* (Milwaukee School of Engineering)
Co-chair: *Meltem Urgun-Demirtas* (Argonne National Laboratory)

2:00 PM Design of Novel Bioink Containing Gelatin-Coated Microspheres for Bioprinting (TuC2a)

Muskan Kanungo (Milwaukee School of Engineering), *Wujie Zhang* (Milwaukee School of Engineering)

A major challenge in tissue engineering is the formation of vasculature in tissue and organs. Recent studies have shown that positively charged microspheres promote vascularization, while also supporting the controlled release of bioactive molecules. This study investigated the development of gelatin-coated pectin microspheres for incorporation into a novel bioink. Electrospray was used to produce the microspheres. The process was optimized using Design-Expert® software. Microspheres underwent gelatin coating and EDC catalysis modifications. The results showed that the concentration of pectin solution impacted roundness and uniformity primarily, while flow rate affected size most significantly. The optimal gelatin concentration for microsphere coating was determined to be 0.75%, and gelatin coating led to a positively charged surface. When incorporated into bioink, the microspheres did not significantly alter viscosity, and they distributed evenly in bioink. These microspheres show great promise for incorporation into bioink for tissue engineering applications.

2:20 PM Biocompatible Peg Diacrylate Hydrogel Nanocomposite Emulsion Scale Down for siRNA Drug Delivery Platforms (TuC2b)

Ruth Negru (Illinois Institute of Technology), *Georgia Papavasiliou* (Illinois Institute of Technology), *Fouad Teymour* (Illinois Institute of Technology), *Marcella Vaicik* (Illinois Institute of Technology)

Biocompatible nanoparticle emulsions (BCNE), synthesized using inverse-phase miniemulsion polymerization, result in the formation of crosslinked poly(ethylene) glycol (PEG) hydrogel nanoparticles dispersed in an organic phase of soybean oil (SO). BCNE may be applied topically or administered through local injection for localized drug delivery, targeting specific, cell-based therapies for which transfection remains a challenge. The use of small-interfering RNA (siRNA) on mature adipocyte cells is one example of this, as siRNA interferes with RNA translation of targeted genes but is challenging to move across the cell membrane due to its large size and negative charge. The naturally-derived, consumable organic phase of BCNE may potentially increase drug-loaded nanoparticle adipocyte interactions and the likelihood for transfection, leading to morphology changes, such as uniocular to multiocular lipid droplets and an increase in the number of mitochondria per cell, which allows for increased cell energy expenditure and decreased lipid storage. To maximize siRNA encapsulation while minimizing the amount of siRNA required to achieve desired drug loading, a BCNE scale-down process was designed. Scale-down from 265 mL to 15 mL BCNE resulted in a significant increase in nanoparticle mass recovery yield of 73.7% from 31.9%, while maintaining an average particle diameter of 92.3 +/- 25.4 nm. Current efforts are aimed at quantifying the efficiency of mature adipocyte transfection through optimization of BCNE crosslink density for sustained drug release and gene silencing

2:40 PM Controlled Release of Cytokines By Biodegradable Toroidal Spiral Particles for Enhancement of Localized CAR-T Cell Therapy (TuC2c)

Abigail Hartzell (University of Illinois Chicago), *Ying Liu* (University of Illinois Chicago)

Previous research of toroidal-spiral particles (TSPs) consists of studies on the formation of TSPs and how this can be used as a therapeutic cellular delivery system for treatments such as islet transplantation and CAR-T cell therapy. We have also developed a biodegradable and biocompatible TSP that is composed of gelatin methacryloyl (GelMA) and Poly (ethylene glycol) diacrylate (PEGDA). Our studies have shown that these TSPs can encapsulate therapeutic cells and cytokines to increase the viability and proliferation of these cells. They have been surgically implanted in mouse models and have shown strong anti-tumor effects. In this study we take a further look into the release of the cytokines from the TSP structure.

The optimal composition of the hydrogel of the TSPs is achieved with consideration of the diffusivity of IL-2 into the hydrogel of the TSP, as the hydrogel mixture of GelMA with PEGDA allows for faster degradation of the TSPs. Here we study the fundamental release mechanisms of IL-2 from the TSP. We take a look at both the cytokines interactions between the encapsulated cells and the TSP itself and how each one plays a role in the cytokines release.

3:00 PM Development of the Cellmag-Carwash System for Isolation of Pure Single Cell Populations (TuC2d)

Brittany Rupp (University of Michigan), *Claire Cook* (University of Michigan), *Emma Purcell* (Stanford University), *Abbie Radomski* (University of Michigan), *Nico Mesyngier* (University of Michigan), *Ryan Bailey* (University of Michigan), *Sunitha Nagrath* (University of Michigan)

Single-cell characterization is becoming increasingly necessary as researchers continue to elucidate the role of cellular heterogeneity in biological processes. While many methods have been proposed to perform single-cell isolation and analysis, droplet microfluidics are optimal technologies because their small scale requires minimal reagents, and they can achieve high throughput. Here we present the CellMag-CARWash droplet microfluidic system and optimized workflow to isolate single natural killer (NK) 92mi cells into single cell droplets. Using anti-CD56 magnetic beads, we were able to achieve >90% specificity and bead attachment to NK cells. After bead attachment, cells are placed into the microfluidic system which uses a magnet to collect cells with beads into droplets while discarding other cells and contaminating material (>95% purity). We experimentally determined that 4 beads per cell is necessary to recover the majority of the cells which is less than the average number of beads per cell (5.3 beads/cell) that attach to NK cells. The resulting droplets can be used to perform single cell analysis and the capture antibody can be changed to isolate any desired cell population. For NK cells, we found the viability of cells in droplets to be >50% after 24 hours. We propose future work that would examine the extracellular vesicles excretion from single NK cells. Extracellular vesicles (EVs) are nanovesicles that are thought to participate in cellular communication. By exposing NK cells to known activators and examining changes in EV secretion, we could develop a more thorough understanding of immune cell communication and function.

Environmental Compliance & Remediation II

Tuesday, March 1, 2022 (**TuD1**)
Chair: *Aditya Prajapati* (Lawrence Livermore National Laboratory)
Co-Chair: *Shri Dawande* (Honeywell UOP)

3:30 PM A Membrane-Based Desalination Technology for Reuse and Recovery of Produced Water (TuD1a)

Hossein Dallalzadeh Atoufi (Illinois Institute of Technology), *David Lampert* (Illinois Institute of Technology)

During the exploration and production of oil and gas, a variety of waste materials are generated. In the oil and gas industry, the most common waste product extracted from hydrocarbon-bearing strata during oil and gas extraction is often called produced water. It includes any chemicals added downhole, or during drilling, production, or maintenance, as well as formation water, and injection water. This waste stream contains significant concentrations of total dissolved solids, dispersed oil and grease, salts, organic compounds, heavy metals, and radionuclides. Often, produced waters are managed on-site or within an oil field using evaporation ponds and seepage pits. Produced waters can also be recycled and reused for exploration and production operations within the oil and gas industry. Produced water management options are currently offered by many vendors, service providers, and water treatment companies. Based on their analysis, the cost of treating produced water, including desalination, is much higher than reusing the produced water in the oil and gas field or injecting it into disposal wells. This research aims to develop a desalination method to reuse and recycle produced water at a lower cost using reverse osmosis. Our reverse osmosis system with polymeric membranes enables us to reach the best efficiency possible. Additionally, this research seeks to recover valuable elements from produced water like lithium to convert waste into valuable materials.

3:50 PM Simulation of Pollutants Distribution for an Impulse Input in Free Streams (TuD1b)

Seyed Javad Amirfakhri (University of Wisconsin – Stevens Point)

Pollutants distribution in free streams such as rivers is an important parameter that affects quality of water, aquatic life, and human health. Pollutants distribution depends on several factors such pollutant specifications, type of input function, kinetics of biodegradation, river dimensions, and velocity of water. Impulse input is a common type of water contamination when a finite amount of a pollutant enters rivers in a short period of time resulting in unsteady state concentration distribution. In this work, Mathematica is used to simulate one dimensional pollutants distribution in rivers for impulse inputs. Three different biodegradation kinetics (Monod, first and zero order) with different biodegradation rate constants are studied. The Peclet number (Pe=L.u/kx) between 0.1 and 1000 is used to study the effect of river dimensions, water velocity, and longitudinal dispersion coefficient (kx). According to the results pollutant concentration drops sharply at low Pe numbers for pollutants with maximum specific degradation rate of 10 mg substrate/(mg biomass.h) and biomass concentration of 250 mg/l indicating that river acts as an ideal CSTR. On the other hand, pollutant concentration vs. length of river decreases gradually at high Pe suggesting that the river can be model as an ideal plug flow reactor. The results indicate that using first and zero order kinetics can lead to misunderstanding of real concentration of pollutants under some conditions.

4:10 PM Defluoridation of Water Using Aluminum Coated Sand Sorbent (TuD1c)

Kiana Modaresahmadi (University of Illinois Chicago), *Amid Khodadoust* (University of Illinois Chicago)

Fluoride has been classified by the World Health Organization (WHO) as a global contamination issue in natural water, where fluoride levels greater than 1.5 mg/L may lead to major health problems such as fluorosis, brain damage, thyroid disease, and cancer. Fluoride can be released and spread throughout the environment due to a variety of causes, including the slow dissolution of fluoride minerals and their host rocks into groundwater, which is one of the most common sources of fluoride contamination, as well as industrial discharge from semiconductor and ceramic manufacturing. The removal of fluoride from water containing high fluoride levels is necessary for providing safe drinking water. Adsorption has been employed as an effective technology for removal of fluoride from water; metal oxide based adsorbents have shown high potential for removal of fluoride. In this study, an aluminum coated sand sorbent was developed as a low-cost adsorbent for removal of fluoride from water with potential application in flow-through water filtration systems. The aluminum coated sand sorbent was able to remove nearly 92 percent of fluoride from water with an initial concentration of 10 mg/L fluoride down to less than 1 mg/L fluoride within six hours. The removal of fluoride by the aluminum coated sand sorbent was due to the adsorption of fluoride onto the aluminum oxide/hydroxide present on the surface of the aluminum coated sand sorbent. The removal of fluoride from water using the aluminum coated sand sorbent was evaluated as function of time, solution pH, and adsorbent dosage.

4:30 PM Design of an Electric Field-Assisted Water-Gradient System for CO2 Capture (TuD1d)

Rohan Sartape (University of Illinois Chicago), *Aditya Prajapati* (University of Illinois Chicago), *Meenesh Singh* (University of Illinois Chicago)

The current industrially relevant CO2 capture technologies either require high maintenance or are energy-intensive rendering them inefficient for long-term use. The water-dependent equilibrium of CO2 with carbonates and bicarbonates in the presence of water can be an alternative to the existing technologies. CO2 can be captured in an environment with hydroxyl ions to convert into bicarbonates which in turn can turn back into carbonates and CO2 in the presence of water. In this work, we exploit this phenomenon by demonstrating a conceptual design of CO2 capture by establishing a gradient of water across an anion exchange membrane by keeping an organic solvent saturated with hydroxyl ions on one side of the membrane and an aqueous solution on the other side. The organic side of the membrane captures CO2 and produces a high concentration of HCO3- diffusing towards the aqueous side, where HCO3- converts back to CO2 for its end-use. To accelerate this process, an electric field is applied to influence the migration of the HCO3- ions. A computational approach to such a process that continuously captures CO2 on the organic side and releases it on the aqueous side will be shown using COMSOL Multiphysics. The various process parameters such as water concentration on the organic side, membrane thickness, feed concentration of CO2, and the applied current density are studied as a part of this work. A working prototype of this system was also developed to show a high CO2 capture flux compared to the currently existing CO2 capture technologies.

Machine Learning & Optimization

Tuesday, March 1, 2022 (**TuD2**)
Chair: *Noah Paulson* (Argonne National Laboratory)
Co-chair: *Hakim Iddir* (Argonne National Laboratory)

3:30 PM Machine Learning for Large Scale Dynamic Systems Based on Model Reduction Technique and Orthogonal Experimental Design Method (TuD2a)

Weiguo Xie (University of Minnesota Duluth)

Process industry plants generate massive volumes of data from numerous devices and sensors, with the data representing a wide range of time and spatial-scales. Unfortunately, most of this data is archived without contributing to the decision-making processes due to a lack of suitable data analysis techniques. Furthermore, in reality it is often very difficult to obtain formulations for those nonlinear dynamic systems. It is necessary to develop dynamic models for those "black-box" systems, and then they can be used for optimization and control. In this research, a machine learning for large-scale dynamic systems has been developed based on model reduction technique and orthogonal experimental design (OED) method. An off-line model reduction technique, the proper orthogonal decomposition (POD) method, is first applied to extract accurate non-linear low-order models from the non-linear dynamic system. A series of successive feedforward artificial neural networks (ANNs) with OED are trained based on the time coefficients of POD basis functions to obtain the dynamic model for the system. POD is based on the spectral theory of compact, self-adjoint operators expressed in the Karhunen–Loève decomposition theorem. POD is a powerful method to catch the most "energy" in an average sense for efficient linear decomposition in terms of data compression. OED is an efficient way for data sampling to study the effect of many factors simultaneously using orthogonal arrays and factor analysis. A benchmark case study for the dynamic oscillatory behavior of a tubular reactor with recycle is used as an illustrative example to demonstrate this methodology.

3:50 PM An Efficient Reinforcement Algorithm Approach to Stochastic Optimal Control with Application to Biodiesel Production (TuD2b)

Shiam Kannan (Vishwamitra Research Institute), *Urmila Diwekar* (Vishwamitra Research Institute)

Stochastic optimal control problems are one of the most difficult problems in optimization. There are very few approaches to solving stochastic optimal control problems in the literature. This paper presents a new and efficient Reinforcement Learning approach to solving stochastic optimal control problems based on the Batch Q-learning algorithm. To improve the convergence of the RL algorithm, we use k-dimensional uniformity of advanced sampling procedures, namely employing the Halton and Hamersley sequences (HSS). These sequences are used to randomly sample the discrete controls from the action space for the RL optimal control problem. The Neural-fitted Q-iterative algorithm is applied to solve an optimal control problem for a first-order state dynamical system. We illustrate the approach using a case study of biodiesel production where kinetics uncertainties result in stochastic optimal control. We present the comparison of our HSS-RL algorithm with that of the stochastic maximum principle.

4:10 PM Accelerated Discovery of Energy Storage Materials Via Multiobjective Bayesian Optimization (TuD2c)

Hieu Doan (Argonne National Laboratory), *Rajeev Assary* (Argonne National Laboratory)

Redox flow batteries (RFBs) are a promising technology for stationary energy storage applications due to their flexible design, scalability, and low cost. In RFBs, energy is carried in flowable redox-active materials (redoxmers) which are stored externally and pumped to the cell during operation. Further improvements in the energy density of RFBs necessitates redoxmer designs with wider redox potential windows and higher solubility. Additionally, designing redoxmers with a fluorescence-enabled self-reporting functionality allows monitoring of the state of health of RFBs. To accelerate the discovery of redoxmers with desired properties, state-of-the-art machine learning methods, such as multiobjective Bayesian optimization (MBO), are useful. Here, we first employed density functional theory calculations to generate a database of reduction potentials, solvation free energies, and absorption wavelengths for 1400 redoxmer molecules based on a 2,1,3-benzothiadiazole (BzNSN) core structure. We utilized these data to develop and benchmark an MBO approach to identify candidates quickly and efficiently with multiple targeted properties. With MBO, optimal candidates from the 1400-molecule data set can be identified at least 15 times more efficiently compared to the brute force or random selection approach. We also applied this approach to an unseen dataset of 1 million BzNSN-based molecules, where we identified several new Pareto-optimal molecules after only 100 evaluations. We anticipate that this active learning technique is general and can be utilized for the discovery of any class of functional materials with multiple desired properties.

4:30 PM Generalized Global Sustainability Model (GGSM) to Study Food-Energy-Water (FEW) Nexus (TuD2d)

Apoorva Nisal (University of Illinois Chicago), *Urmila Diwekar* (Vishwamitra Research Institute), *Neeraj Hanumante* (Indian Institute of Technology Bombay), *Yogendra Shastri* (Indian Institute of Technology Bombay), *Heriberto Cabezas* (University of Miskolc)

Inordinate consumption of the natural resources by humans over the past century and unsustainable growth practices have necessitated a need for enforcing global policies to sustain the ecosystem and prevent irreversible changes. A global model has been developed recently with focus on sustainability for the Food-Energy-Water (FEW) Nexus (Nisal et al, 2021; Hanumante et al, 2021). This model is a 15-compartment model with components for the food-web, microeconomic framework, energy, industry and water sectors and, humans. Model development is done using global-scale data for stocks and flows of food, energy, and water. It was validated based on historical data for global sectors and has the capacity to predict population, global and regional water stress, GHG emissions and the gross domestic product (GDP) for the next century. Moreover, the model can consider the production of renewable energy using biofuels (biopower). Baseline results show that the model is stable. Further analysis of several scenarios to evaluate sustainability with this model showed that indiscriminate human consumption would lead to collapse of several resources in the future. An exponential increase in the human population exacerbates this process with the resources getting exhausted sooner. Water stress on the global and regional levels is then projected and net water stress is used for evaluation. Results show that available global water is adequate to support the rising demand in the next century, but regional diversity of water availability leads to high stress in Africa. Future work includes an optimal control based approach to maximize sustainability.

Poster Session

Tuesday, March 1, 2022 (**TuP1**)
Chair: *Karthika Suresh* (University of Illinois Chicago)

5:00 PM Poster Session

Poster 1 **WITHDRAWN (TuP1c)**

Poster 2 **Understanding the Mechanisms and Feasibility of Solar-Radiation-Enhanced Ammonia Synthesis (TuP1d)**

Carissa Yim (University of Michigan), *Alexander Hill* (University of Michigan), *Johannes Schwank* (University of Michigan), *Andrej Lenert* (University of Michigan)

Energy-conscious methods for ammonia (NH3) synthesis are imperative to reduce its 1-2% contribution to global CO2 emissions. Currently, the Haber-Bosch process relies on hydrogen production by steam reforming and is thus a centralized process, causing access inequity for resource-constrained communities. Renewable hydrogen and novel catalysts that can achieve favorable kinetics and thermodynamics under milder reaction conditions are necessary for distributed NH3 production. To meet these challenges, electromagnetic irradiation can be coupled with heat to (1) overcome high activation energy barriers and (2) enable smaller, modular, and distributed NH3 synthesis systems. Renewable hydrogen generation by water-electrolysis can also be used to supplant conventional steam methane reforming and strive toward carbon-free NH3 synthesis.

To achieve renewable-energy driven, distributed NH3 systems, we must understand how sunlight and heat in tandem affect reaction pathways and accelerate NH3 formation over a catalyst. Thanks to substantial, established literature on CO2 behavior on catalytic surfaces, CO2 can be used as a simple model system to set the stage for NH3 experiments. As such, we will examine how light influences reaction-intermediate interactions with Ru/TiO2 catalysts through diffuse reflectance infrared spectroscopy (DRIFTS) using CO2 reduction as a probe. Learning the mechanism of photo-enhanced thermal catalysis provides a foundation to harness solar energy through novel reactor design and ultimately deliver distributed, green-ammonia to resource-constrained communities. Looking ahead, we seek to address application scale considerations such as the intermittency of sunlight, light coupling into the reactor, and scaling of the auxiliary components of our proposed plant design.

Poster 3 **An Evaluation Method for Energy Performance of Sulfur Recovery Units and Tail Gas Treatment Units Based on Grey Correlation Analysis (TuP1f)**

Min Qiu (China University of Petroleum, Beijing), *Zhongli Ji* (China University of Petroleum, Beijing), *Limin Ma* (China University of Petroleum, Beijing)

In the purification process of natural gas with high sulfur content, sulfur recovery units are mostly used in conjunction with tail gas treatment units. A large amount of fuel gas is consumed in the process, which is also accompanied by the recovery and utilization of waste heat. In order to evaluate the energy consumption performance of the sulfur recovery unit and the tail gas treatment unit during actual operation, a comprehensive evaluation model of the units' operational performance based on grey correlation analysis is established. Firstly, the influence weights of the evaluation indicators in the model are determined based on the historical operation data of the units, combined with partial correlation analysis. Then, the BP neural network and NSGA-II algorithm are used to determine the benchmark operating conditions of the units. Finally, the evaluation result of the energy consumption performance of the units is achieved by calculating the correlation degree under the actual operating conditions. The proposed model provides directions for optimizing the operation of the units while achieving an evaluation of the operational performance.

Poster 4 **Experimental Investigation on the Gas–Liquid Separation Performance of Vane Separators with Bio-Inspired Functional Surfaces (TuP1g)**

Jiarong Wang (China University of Petroleum, Beijing),
Zhongli Ji (China University of Petroleum, Beijing),
Wenchao Lu (China University of Petroleum, Beijing),
Yufeng Liu (China University of Petroleum, Beijing)

Vane separators are widely used in natural gas purification processes to remove entrained fine water particles from the main gas flow. In this work, several aluminum alloy surfaces with different wettability are prepared by chemical etching, boiling water treatment and low-surface-energy material modification. The effects of surface wettability on the separation efficiency and pressure drop have been experimentally studied by liquid mass balance methods. The results show that the separation efficiency of the vane separator with high hydrophobicity is the highest among all the samples with uniform wettability at the same operating conditions. Furthermore, the bio-inspired functional surfaces with wettability gradient can remarkably improve the separation efficiency of vane separators. However, the pressure drop is hardly affected by the surface wettability because the shapes of flow channels remain unchanged.

Poster 5 **Computational Study of on-Surface and Sub-Surface Oxygen in Rh(111) (TuP1h)**

Weronika Walkosz (Lake Forest College), *Emma Remish* (Lake Forest College), *Juan Garcia* (Argonne National Laboratory), *Hakim Iddir* (Argonne National Laboratory), *Daniel Killelea* (Loyola University Chicago)

Various properties of metal surfaces can be altered by interactions with oxygen, which can reside on the metal surfaces as well as in the subsurface region. It has been shown that subsurface oxygen greatly affects the reactivity of catalytic surfaces and is a precursor for oxide formation. Using Density Functional Theory calculations, we investigate various structures of O on the (111) surface of Rh as well as the competition between oxide formation and dissolution of oxygen into Rh to form subsurface oxygen. We find that surface O prefers to bind at the surface fcc site of Rh(111) at a coverage of 0.25 ML, but the binding energy decreases with increasing O coverage. In the subsurface region, the oxygen's preferred binding site is the tetra I site, but the subsurface binding is less favorable than the on-surface binding at 0.25 ML. We also considered arrangements involving structures with combined surface and subsurface O atoms to identify which structures are energetically favorable at higher coverage. Furthermore, we focused on identifying pathways for surface diffusion of low-coverage adsorbed atomic O between different sites on Rh(111) as well as the surface to subsurface diffusion. The obtained results are expected to further our understanding of the chemistry of transition metal surfaces and their importance in heterogeneously catalyzed reactions.

Poster 6 **Impact of Anion Species in the Biosorption of Nickel and Lead By *Lemna m*.**

Magdalene Jones (University of Minnesota Duluth),
Steven Sternberg (University of Minnesota Duluth),
Robert Licari (University of Minnesota Duluth)

Multiple water quality challenges are created by mining. Of these, heavy metal contamination is one of the most prevalent. This study examined the impact of anions, associated with the water, have on the ability of *Lemna m*. (duckweed) to remove those heavy metals. We examined the removal potential and kinetics of the uptake of Nickel and Lead by *Lemna m*. in the presence of Carbonate, Sulfate, Nitrate, and Chloride using lab-scale batch reactors. *Lemna m*. removed Lead from water at 70.9%±4.2, 89.5%±0.7, 88.8%±0.9, 88.1%±0.2, and 92.3%±0.03 in the presence of Sulfate, Nitrate, Chloride, Carbonate (tap water), and DI water respectively. Nickel was removed at 22.2%±2.6, 28.2%±10, 14.3%±3.1, and 31.2%±2 for Sulfate, Nitrate, Chloride, and DI water This study coincides with the MNDrive goal of using aquatic plants to reduce heavy metal concentrations in mining wastewater. The funding source, MNDrive, was Minnesota's Discovery, Research, and InnoVation Economy, Undergraduate Research Scholars program.

Poster 7 **Machine Learning Prediction of Hydration and Ion Association Properties of Zwitterions**

Daniel Christiansen (University of Illinois Chicago),
Steven Sternberg (University of Illinois Chicago), *Robert Licari* (University of Illinois Chicago)

Applications of machine learning (ML) in material design have become prolific due to advances in computing power, software availability, and novel public datasets of material properties. However, these often have difficulty modeling polymeric materials due to the diversity of potential formulations and processing conditions, multiscale physics, and scarcity of well-developed polymer property datasets. Given these materials ubiquity in our world, it is critical that these problems are addressed. Recently published works suggest these challenges may be mitigated by incorporating lower-scale features, defining material composition and physics, into the training data for higher-scale ML models. This hierarchical ML (HML) scheme has been used to accurately predict macroscopic polymer properties by including lower-scale features from physical equations and simulations. In this work, we present the first tier of an HML scheme to predict ionic conductivity of zwitterionic polymer hydrogels. Specifically, this work examines the "microscopic" scale, where the hydration and ion association properties of 240 zwitterions are studied by molecular dynamics simulation. The coordination shell radii, coordination number, and effective residence time are calculated and used as target variables for ML. Cheminformatic descriptors, detailing chemical and physical properties, and system descriptors are used to train highly accurate ML models. With these models, it is possible to predict the microscopic-scale features of zwitterions from chemistry alone and will accelerate future studies of these materials by avoiding costly computational simulations. These data and models will be used as inputs for training higher-scale ML models to predict properties of single- and multi-polymer zwitterionic systems.

Local Section Dinner and Dinner Keynote
Tuesday, March 1, 2022 (**TuK3**) [**Zoom signup link**]

7:00 PM Diversity, Perfect Mixing, Symmetry, and Autocatalysis: Random thoughts on celebrating differences.
Fouad Teymour (Illinois Institute of Technology)

An informal tour of the personal and professional observations of a chemical engineer and theater artist about diversity in nature, society, and engineering, told through stories, anecdotes, video clips, and research article results.

Presentation Abstracts (Day 2)

Wednesday, March 2, 2022

Wednesday Morning Keynote Session
Wednesday, March 2, 2022 (**WeK1**)

8:35 AM The Blue and Green Energy Translation

Henrik Rasmussen (Haldor Topsoe)

The presentation will detail the current trends in green and blue Hydrogen, ammonia and methanol for the new energy transition from fossil to blue and green energy sources. We will also discuss the production technology options for each product. The presentation will also discuss the advantages of Solid Oxide Electrical Cell technology (SOEC) over Alkaline electrolysis for the production of green H2.

Refining & Renewables
Wednesday, March 2, 2022 (**WeA1**)
Chair: *Belma Demirel* (bp)
Co-Chairs: *Hadjira Iddir* (Becht), *Meltem Urgun-Demirtas* (Argonne National Laboratory)

9:40 AM Why and How Refineries Will Drive the Transition from Fossil to Renewable Fuels (WeA1a)

Peter Nymann (Haldor Topsoe)

Renewable carbon-based feedstocks come in many forms and from many different sources. They all need extensive processing involving hydrotreating, cracking and dewaxing before they can be applied as renewable transportation fuels or as precursors for production of renewable petrochemicals. The refineries have the infrastructure and equipment to undertake this treating, and Topsoe has identified the challenges and opportunities connected with this tremendous task. The renewable feedstocks may be co-processed in existing units or processed in stand-alone units based on revamped existing units or newly designed grassroot units. The optimal choice of where to process these streams depends on the desire for Sustainable Aviation Fuels (SAF), renewable diesel or precursors for plastic or petrochemicals production. The presentation will give an overview of pros and cons of the potential solutions and challenges with focus on producing SAF.

10:00 AM Unlocking the Potential of Existing Hydrotreaters for Processing Renewable Feedstocks (WeA1b)

Aline Bueno (Albemarle)*, Lucia Basile* (Albemarle)

Co-processing biofuels in diesel hydrotreaters is a proven technology that allows refiners to capture value from existing assets while meeting current renewable fuels standards. Albemarle has provided refiners with catalyst solutions and technical expertise in over 40 biofuels co-processing cycles that have run with a wide variety of feedstocks and operating conditions.

Renewable fuels regulations can be an opportunity for a refiner to minimize environmental impact while increasing profitability if they can act quickly, operate with flexibility, and minimize capital investment. Within the context of supporting customer units, Albemarle has been on the frontline of developing and optimizing catalyst technologies and operational understanding for processing maximum renewable feed sources through existing hydrotreating units.

Albemarle has worked closely with customers since 2008 to optimize catalyst loading design and unit operation to steadily increase co-processing up to 25% in volume with minimum impact on cycle length and refinery turnaround strategy. More recently, Albemarle has executed long-term test runs with customers to process 100% renewables with up to 35% fresh feed intake in an existing unit.

This paper builds on the experience that Albemarle has amassed in renewables, using examples that demonstrate application of our knowledge to avoid pitfalls commonly encountered when processing increased amounts of biofuels. As well, it shows how it is possible to preserve operating flexibility in renewables co-processing operations without the need for capital investment.

10:20 AM Life Cycle Greenhouse Gas Implications of Blending Performance-Enhancing Bioblendstocks at Refineries: Integrated Refinery Optimization and Life Cycle Analysis (WeA1c)

Troy Hawkins (Argonne National Laboratory), *George G. Zaimes* (Argonne National Laboratory), *Yuan Jiang* (Pacific Northwest National Laboratory), *Nicholas Carlson* (National Renewable Energy Laboratory), *Ben Young* (Eastern Research Group), *Andrew Beck* (Eastern Research Group), *Shuyun Li* (Pacific Northwest National Laboratory), *Michael Talmadge* (National Renewable Energy Laboratory) and *Avantika Singh* (National Renewable Energy Laboratory)

Changes to transportation and the broader economy to reduce greenhouse gas emissions in an effort to mitigate global climate change will entail significant changes for the petroleum refining industry. Modifications to refinery operations to meet changing market demands involve dynamic impacts on the processing involved in the production of the various refinery products. To understand the energy and environmental impacts of these changes, we have developed an integrated modeling approach coupling economic optimization of refinery operations using Aspen PIMS with environmental life cycle analysis using the Refinery Products Life Cycle Analysis (RP-LCA) tool to characterize and track environmental impacts across the life cycle of petroleum products. In this study, we consider the potential for improving refinery economics and sustainability by blending biomass-derived bioblendstocks with advantageous fuel properties. We find that while the bioblendstocks have the potential to achieve significant greenhouse gas reductions, these benefits come with a large range of associated marginal carbon dioxide abatement costs. This analysis demonstrates the potential for the RP-LCA tool to help promote more sustainable refinery operations by providing a robust, transparent, and modular framework capable of analyzing greenhouse gas reductions both gate-to-gate within the refinery, at the detailed subprocess level, and across the full life cycle of fuels produced from petroleum and biomass.

10:40 AM Life Cycle Analysis of Plastic to Fuel and Plastic Circular Economy (WeA1d)

Ulises R. Gracida-Alvarez (Argonne National Laboratory), *Pahola Thathiana Benavides* (Argonne National Laboratory), *Uisung Lee* (Argonne National Laboratory), *Michael Wang* (Argonne National Laboratory)

The large flows and short use phase of much of the plastic products (post-use plastic [PUP]) represent an opportunity to produce valuable chemicals and fuels. Life cycle analysis (LCA) can be used to assess the potential benefits of PUP conversion technologies. Therefore, this study presents an updated LCA of pyrolysis of PUP to produce pyrolysis oil and ultra-low sulfur (ULS) diesel and a preliminary analysis on plastics upcycling. For the first part, we collected data from eight pyrolysis companies which was aggregated based on plant capacity (pioneer, Nth-plants, and highest capacity). We used the Greenhouse gases, Regulated Emissions, and Energy use in Technologies (GREET®) model to assess the greenhouse gas (GHG) emissions, fossil energy, and water consumption associated with the production of the pyrolysis products. The LCA results from pyrolysis oil and PUP-derived ULS diesel were compared with those for their conventional counterparts such as petroleum naphtha and petroleum ULS diesel, respectively. The results varied significantly depending on the coproduct treatment method (displacement, energy, and market allocation) and the plant capacity. Most of the reductions in GHG emissions, fossil energy, and water consumption were achieved in the highest capacity plant, which indicates that economies of scale benefit the environmental performance of PUP-derived pyrolysis products. Recently, multiple initiatives have promoted circular economy strategies of PUP to pursue sustainable growth of products and services in the plastic industry. For the second part of this study, we included preliminary results considering the conversion of pyrolysis oil to plastic precursors and new plastic polymers.

Climate Solution: Action I

Wednesday, March 2, 2022 (**WeA2**)
Chair: *Dennis O'Brien* (Advisian)

9:40 AM Greenhouse Gas Emissions at the Metropolitan Water Reclamation District of Greater Chicago (WeA2a)

Joseph Kozak (Metropolitan Water Reclamation District of Greater Chicago), *Jonathan Grabowy* (Metropolitan Water Reclamation District of Greater Chicago)

In recognition of the negative impacts of climate change, the Metropolitan Water Reclamation District of Greater Chicago (District) has adopted a resolution and is working to adopt a Climate Action Plan which includes targeted goals to reduce the organization's carbon footprint. The District's carbon footprint includes both direct emissions as well as indirect emissions from electricity use (Scopes 1 and 2). These reductions are also echoed in the District's 2021-2025 Strategic Plan, where the goal is a 28 percent from the 2005 baseline by 2025 and an 80 percent by 2050. The District's 2020 footprint is 40 percent lower than the 2005 baseline. Further reductions will be achieved through decommissioning our Imhoff tanks, increasing energy efficiencies of facilities, and optimization of plant processes.

10:00 AM Improved Bio-chemical Utilization of Indoor, Aquaponic Growing Systems (WeA2b)

Blake Davis (Illinois Institute of Technology)

Most indoor, aquaponic systems are currently recirculating aquaponics systems (RAS). These arrangements continually recirculate nutrients throughout the system but do not optimize all the chemical and biological processes involved. This presentation will cover the growth of the indoor, controlled-environment agriculture sector and lay out novel solutions to optimizing the chemical and biological processes in indoor, aquaponic growing systems.

10:20 AM The Changing Energy Storage Landscape (WeA2c)

George Crabtree (University of Illinois Chicago/Argonne National Laboratory)

Energy *storage has gone through many* transformations, from powering personal electronics, to enabling decarbonization of passenger electric vehicles (EVs) to providing stabilization of a renewable electric grid against variation due to passing clouds and gusty winds, and to extension of solar generation to meet the evening peak demand. Climate change and decarbonization bring new scope and urgency to energy storage, transforming it from an opportunity to a necessity. In addition to battery energy storage, chemical energy storage to replace fossil fuels remains a significant challenge. The current status and outlook for energy storage in this evolving landscape will be discussed.

Catalysis & Reaction Engineering I

Wednesday, March 2, 2022 (**WeB1**)
Chair: *Trevor Lardinois* (Exponent)
Co-Chair: *Belma Demirel* (bp)

11:10 AM Catalytic Hydrogenolysis of Polyolefin Waste to Higher Value Liquid Products (WeB1a)

Ryan Hackler (Argonne National Laboratory), *Robert Kennedy* (Northwestern University), *Magali Ferrandon* (Argonne National Laboratory), *Massimiliano Delferro* (Argonne National Laboratory)

Catalytic hydrogenolysis of polyolefins was explored using Pt nanoparticles decorating a strontium titanate (STO) support as prepared via atomic layer deposition (ALD) and surface organometallic chemistry (SOMC). Pre- and post-consumer polyethylene and polypropylene of varying structure and molecular weight was evaluated under different reaction conditions to determine the viability of catalytic hydrogenolysis for upcycling a mixed plastic feedstock into a homogeneous product. The resulting products were consistently small (Mw < 1000) and narrow (Đ ≤ 1.6) waxes and liquids, where degree of branching remained unchanged between reactant and product. These high-quality liquids (HQLs) were found to behave similarly to industrial lubricants, with a reduction in wear by 44% compared to standard Group III mineral oils. Performance of plastic-derived HQLs was found to be comparable to expensive synthetic polyalphaolefin (PAO) oils. Furthermore, HQLs were found to synergistically reduce friction and wear when blended into PAOs, both at room temperature and 100 °C, suggesting an ease of implementation into existing lubricant formulations. This work highlights an economically viable method for converting cheap plastic waste into higher value products.

11:30 AM Non-Oxidative Dehydroaromatization of Long-Chain Alkanes on Intermetallic Surface (WeB1b)

Ranjan Behera (Iowa State University), *Wenyu Huang* (Iowa State University)

Dehydrogenation of long chain alkanes have attracted considerable interest from an industrial point of view for the production of fine chemicals. However, thermodynamic constraints such as high temperature and low product selectivity due to various side reactions have been challenging in developing novel catalytic systems. Bimetallic catalysts have been investigated to address the above problems. Here, we have demonstrated Pt-based intermetallic nanoparticles (iNPs) as a highly active and, more importantly, selective catalyst for non-oxidative dehydrogenation of long-chain alkanes to aromatized products of benzene-toluene-xylenes (BTX) family. At a reaction temperature of 550 °C, the intermetallic catalysts have shown superior activity and selectivity compared to monometallic Pt. For the dehydrogenation of C6-C8 linear chain alkanes, the intermetallic catalysts yield BTX selectivity of 88, 92, and 93%, respectively. Kinetics of n-hexane dehydroaromatization, including activation energy calculations, have shown that the reaction barrier is much lower on the intermetallic surface than Pt surface. First-order dehydrogenation kinetics models have demonstrated that the deactivation constant on Pt surface is one order of magnitude higher than that of the intermetallic catalysts. Overall, these results have provided a pathway for developing novel bimetallic catalysts for efficient and selective dehydrogenation processes.

11:50 AM Assessment of Catalysts for Oxidative Coupling of Methane and Ethylene (WeB1c)

Jordy Ramos-Yataco (Northwestern University), *Justin Notestein* (Northwestern University)

Oxidative coupling of methane (OCM) is a direct route to upgrade methane to higher value hydrocarbons in the presence of an oxidant. This work focused on role of the promoter cation in A2WO4-MnOx/SiO2 (A=none, Li, Na, K, Rb, Cs), in particular to establish their behavior at high methane conversions such as would be needed for industrial adoption. Within these, K and Rb presented a similar OCM performance to the more popular Na. Other systems were evaluated, including a Ag-doped catalyst that did not impact yield but did increase the formation of C3+, and a boron-based catalyst that is attracting attention for related reactions but which was much less selective to C2+. We also established that La co-doping on A2WO4-MnOx/SiO2 had a minimal impact on C2+ formation, in contrast with other reports. Overall, many claims of exceptional performance or important crystalline compositions did not hold up under high-conversion conditions. Finally, it was noted that ethylene and propylene concentrations rose in proportion. As such, the effect of ethylene-methane co-feeds were also investigated over Na2WO4-MnOx/SiO2. This promoted COx formation but also increased the C3+ selectivity, which may be of interest under certain operating scenarios.

Climate Solution: Action II

Wednesday, March 2, 2022 (**WeB2**)
Chair: *Dennis O'Brien* (Advisian)

11:10 AM Material Flow Analysis of Polyurethane (WeB2a)

Chao "Chloe" Liang (Northwestern), *Jennifer Dunn* (Northwestern)

Today, polyurethanes are effectively not recycled and are made principally from non-renewable, fossil-fuel derived resources. Our work provides the first high-resolution material flow analysis (MFA) of polyurethane flows through the U.S. economy, tracking back to fossil fuels and covering polyurethane-relevant raw materials, trade, production, manufacturing, uses, historical stocks, and waste management. This MFA study provides a panoramic view of the current polyurethane system and tracks with detail the life trajectory of each polyurethane type and polyurethane-containing end-use product, which can be used as a powerful tool to identify the most impactful chemicals for the product of interest and direct redesign efforts. In addition, the depicted polyurethane map reflects the baseline scenario that could help determine the challenges and opportunities of recycling and sustainability, guide development focuses of related technologies, and support stakeholders in building a more circular and sustainable polyurethane system.

11:30 AM Nuclear Energy and Energy Sustainability: Resources, Environment and Climate (WeB2b)

Pavel Tsvetkov (Texas A&M)

This talk will discuss contemporary developments in nuclear energy in relation to the context of sustainably. Resources, environmental considerations and impact, and climate considerations will be in the center of the discussion. Together with renewable energy sources, nuclear energy has a potential to become the key energy source for the future. While not inherently renewable, nuclear energy is inherently sustainable as it is the only energy source that has capability to “reproduce” itself. Advantages, opportunities, and challenges associated with nuclear technologies will be discussed.

11:50 AM WITHDRAWN (WeB2c)

Wednesday Afternoon Keynote Session

Wednesday, March 2 2022 (**WeK2**)

1:05 PM An atomic-scale perspective on catalyst’s stability and on the nature of the active site when the reaction is taking place

Manos Mavrikakis (University of Wisconsin-Madison)

Addressing the question of the nature of the active site has been a central challenge in various types of catalysis (thermal heterogeneous, electrocatalysis, etc.) for a long time. With the advent of modern instrumentation providing atomic-scale information about catalytic surfaces, including under reaction conditions, and powerful spectroscopies combined with ever-increasing computational speed enabling extensive electronic structure calculations, addressing the question on the nature of the active site has become more viable. In this talk, we will discuss examples of catalytic reactions, whereby a combination of reaction kinetics and characterization experiments with microkinetic modeling, informed by first-principles calculations, allows the derivation of insights on: (i) reaction mechanism at the elementary step level and (ii) the nature of the active site when the reaction is taking place. The role of spectator species versus active intermediates turning reactants over to products will be elucidated.

The second objective of this talk is to discuss catalyst’s stability, a property equally important to its activity and selectivity, and which often determines whether a catalytic process becomes financially viable or not.

Catalysis & Reaction Engineering II

Wednesday, March 2, 2022 (**WeC1**)
Chair: *Trevor Lardinois* (Exponent)
Co-Chair: *Belma Demirel* (bp)

2:10 PM Highly Selective Atomically Dispersed Copper Electrocatalyst for CO2 Reduction to Ethanol (WeC1a)

Haiping Xu (Argonne National Laboratory)

Ethanol has been extensively blended in gasoline as fuel to improve the combustion efficiency. Electrochemical CO2 reduction reaction (CO2RR) to ethanol and other value-added chemicals offers a promising “carbon-neutral” or even “carbon-negative” strategy when combined with renewable electricity, making the approach not only environmentally sound but also economically attractive. A key challenge for CO2RR is the lack of electrocatalyst that is capable of converting CO2 to a single product with high current efficiency, i.e. Faradaic efficiency (FE), low overpotentials and high durability.

Here, we report the preparation of commercial carbon-supported Cu SA catalysts by an amalgamated Cu–Li method. The catalysts demonstrated highly selective CO2-to-ethanol conversion with FE reaching ~91% at -0.7 V versus RHE and an onset potential as low as -0.4 V with FE of ~15%. The FE of the catalysts maintained at roughly 90% without degradation for 16 h. The CO2-to-ethanol FE is favored by high initial dispersion of single Cu atoms. Operando synchrotron X-ray absorption spectroscopy revealed that such dispersion played a critical role in a reversible transformation between Cu SA and Cun (n= 3 and 4) as the active sites during the electrocatalytic reaction. Understanding the role of metal single atoms on the CO2 electrochemical reduction reaction is fundamentally important in designing new CO2RR catalyst for the large-scale production of value-added liquid fuels and chemicals.

2:30 PM Bimetallic Ru-Based Alloy Nanoparticles: Unravelling the Effects of in Addition on Methanol Synthesis from CO2 (WeC1b)

Feiyang Geng (University of Notre Dame), *Jason Hicks* (University of Notre Dame)

Carbon dioxide (CO2) hydrogenation has continued to receive significant attention as an effective route to recycle CO2 into usable products, such as methane, CO and methanol. CO2 hydrogenation to methane is the most feasible pathway among the three products from a thermodynamic perspective (<500 oC). However, methanol is a more valuable platform chemical. Yet, the identification of new catalyst compositions that avoid methane formation while maximizing methanol yields remains a significant challenge.

Ruthenium is one of the most active and selective catalysts for CO2 methanation. Efforts to modulate the selectivity of Ru-based catalysts for methanol synthesis have been made through the development of homogeneous, molecular catalysts; however, these catalysts often suffer from limited thermal stabilities and difficulties separating from the product to reuse/recycle. An alternative approach is through the formation of a bimetallic alloy, which alters the catalyst performance through electronic and geometric effects. This approach has been successful with In-Pd alloys to prohibit the CO methanation pathway.

In this study, we evaluated In-Ru alloys for liquid phase CO2 hydrogenation. Our work showcases that incorporation of indium promotes methanol selectivity to 86%, and prohibits methane production at 240 oC where pure Ru produced 98% methane. In addition, we performed diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) experiments, CO TPR, H2-D2 exchange. These experiments provide further insight into the role of In in tuning the interaction between surface species (formate, methoxy, CO and hydrogen) and surface sites, leading to better methanol selectivity than pure Ru

2:50 PM First-Principles Analysis of the Ammonia Decomposition Reaction on High Entropy Alloy Catalysts (WeC1c)

Zuhal Cakir (Purdue University), *Liangbing Hu* (University of Maryland), *Chao Wang* (Johns Hopkins University), *Jeffrey Greeley* (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, known as 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 subsequently extending these ideas to incorporate multiple elements. Additionally, 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 development of high entropy alloy catalysts for ammonia decomposition.

3:10 PM WITHDRAWN (WeC1d)

<u>Energy Storage I</u>

Wednesday, March 2, 2022 (**<u>WeC2</u>**)
Chair: *Hakim Iddir* (Argonne National Laboratory)
Co-Chair: *Juan Garcia* (Argonne National Laboratory)

2:10 PM A Unique Co-Free Cathode for High Energy Li-Ion Cells (WeC2a)

Boyu Shi (Argonne National Laboratory), *Jihyeon Gim* (Argonne National Laboratory), *Linze Li* (Pacific Northwest National Laboratory), *Chongmin Wang* (Pacific Northwest National Laboratory), *Anh Vu* (Argonne National Laboratory), *Jason R. Croy* (Argonne National Laboratory), *Michael M. Thackeray* (Argonne National Laboratory), *Eungje Lee* (Argonne National Laboratory)

A new Li-ion battery cathode, 'LT-LiMn0.5Ni0.5O2', where LT refers to its relatively low synthesis temperature (400 °C), has been identified. Electrochemical data indicate that Li/ LT-LiMn0.5Ni0.5O2 cells operate between 5.0 and 2.5 V with good cycling stability, yielding a cathode capacity of 225 mAh/g. The electrochemical reactions occur in two distinct steps centered at ~3.75 V and ~4.7 V during charge, and at ~4.6 V and ~3.5 V during discharge. Highangle, annular-dark-field (HAADF) scanning-transmission electron microscopy (STEM) provide evidence that LT-LiMn0.5Ni0.5O2 consists of a unique, partially-disordered LT-LiMn0.5Ni0.5O2 structure with predominant lithiated-spinel- and layered-like character. Structural analysis of LT-LiMn0.5Ni0.5O2 with synchrotron X-ray diffraction data shows, surprisingly, that lithiated-spinel and layered models with approximately 16% (~1/6) disorder between the lithium and manganese/nickel ions, yield an identical fit to the data, complicating the determination of the exact nature and level of disorder in each structural model. We believe that this is the first report of a Mn-stabilized, lithium-nickel-oxide spinel-related structure in which the redox reactions occur almost entirely on the nickel ions, with the likelihood that oxygen redox also contributes to some capacity above 4.7 V.

2:30 PM Insights from Computational Studies on the Anisotropic Volume Change of LixNiO2 at High State of Charge (x < 0.25) (WeC2b)

Juan Garcia (Argonne National Laboratory), *Joshua Gabriel* (Argonne National Laboratory), *Noah Paulson* (Argonne National Laboratory), *John Low* (Argonne National Laboratory), *Marius Stan* (Argonne National Laboratory), *Hakim Iddir* (Argonne National Laboratory)

The need for high-capacity Li-ion battery cathodes has favored the increase of Ni content in commercial battery cells. However, at high state of charge (SOC), Ni-rich materials undergo a phase transition and volume collapse with deleterious effects on battery performance. It is uncertain whether this drastic volume change is caused by the phase transition or not. To provide more insight into the volume-phase transition relationship in the high Ni cathode LixNiO2, we performed density functional theory calculations, along with molecular dynamics simulations using machine learned potentials to calculate the temperature and composition dependent free energy differences between the suspected phases at high state of charge (x<0.25). We find that the calculated free energy difference between the suspected phases containing different oxygen stacking sequences is small at room temperature. Further, we find that the collapse of the layered LiNiO2 c-lattice parameter at high SOCs is mainly due to the electronic depletion of the oxygen sublattice and the lack of screening from positive Li ions. The interactions between adjacent oxygen ions across an empty Li layer (NiO2), are largely controlled by Van de Waals interactions and are in fact similar regardless of the oxygen stacking—which explains the negligible free energy differences between O1 and O3 stacking in NiO2

2:50 PM Probing the Impedance at Low States of Charge in Li- and Mn-Rich Oxides (WeC2c)

Arturo Gutierrez (Argonne National Laboratory)

materials for lithium-ion batteries has brought the focus of the research community back to Li- and Mn-Rich oxides (LMR). These oxides remain attractive because of the high specific capacities they deliver as well as the economic benefits they offer by replacing more expensive nickel-based chemistries with Mn-rich (>50%) compositions. But, in order to enable deeper market penetration, several unresolved challenges should be addressed. Principal among those challenges is a premature rise in area-specific-impedance (ASI, Ω·cm2) at low states of charge, denoted hereafter as ΩLSOC. Harmful effects of ΩLSOC in LMR-NMC include limiting accessible capacities at high rates of discharge, therefore, negating some of the advantages of high specific capacities.

This presentation will discuss recent work led by Argonne National Laboratory that has contributed to further understanding the root causes/mechanisms leading to ΩLSOC. The effect of surface, bulk, and morphological contributions to the impedance behavior of LMR-NMC will be presented.

3:10 PM Electrolyte Engineering to Stabilize Cathode-Electrolyte Interface of Na1-XFeO2 Cathode for Na-Ion Batteries (WeC2d)

Jehee Park (Argonne National Laboratory), *Kyojin Ku* (Hanbat National University), *Seoung-Bum Son* (Argonne National Laboratory), *Jihyeon Gim* (Argonne National Laboratory), *Youngsik Kim* (Ulsan National Institute of Science and Technology), *Eungje Lee* (Argonne National Laboratory), *Christopher Johnson* (Argonne National Laboratory)

Na-ion batteries have received extensive attention in recent years with the growing demand of sustainable energy storage systems for grid-scale applications. [1] Numerous efforts have been conducted to develop the new electrode materials for Na-ion batteries toward cost-effectiveness, high energy density, and long cycle life. Iron(Fe)-based layered cathodes could be one of the most promising candidates because iron is an earth-abundant, low-cost, environmentally benign element, and stable in a layered structure. [2] As a prototype material, layered NaFeO2 cathode is electrochemically active associated with the Fe3+/Fe4+ redox reaction, which provides a high operating voltage (~3.3 V) and energy density (~300 mWh/g). [3] However, since Fe4+ is not common oxidation state for iron, a parasitic side reaction between unstable Fe4+ species and the electrolyte occurs resulting in a significant degradation process that is not fully understood. [4] Therefore, investigation of the cathode-electrolyte interface and reactivity of NaFeO2 is essential in order to develop efficient strategies and improve battery performance.

Herein, we investigated the electrolyte effect on the side reaction of Na1-xFeO2 cathode and have improved the cathode-electrolyte interface by electrolyte modification. The addition of fluoroethylene carbonate additive along with NaPF6 salt suppressed the side reaction and improved the reversible capacity, coulombic efficiency, and cycling stability. We will present these findings and discuss their implications on the Fe-based layered oxide cathode for future development.

<u>Fluid Properties, Fluid Dynamics, & Transport Phenomena</u>

Wednesday, March 2, 2022 (**<u>WeD1</u>**)
Chair: *Robert Tsai* (Honeywell UOP)
Co-Chair: *Karthika Suresh* (University of Illinois Chicago)

3:40 PM Development on Measurement Technology for Studying Mixing and Reaction State Using Online Electrical Resistance Tomography (WeD1a)

Braden Hoff (University of Minnesota Duluth), *Weiguo Xie* (University of Minnesota Duluth)

Electrical resistance tomography (ERT) has been applied in a wide range of scientific and engineering fields, such as geophysical study, clinical diagnosis, chemical or mineral process measurement, and process optimization. ERT is usually used to collect data on the processes in vessels and pipes. In this research, ERT uses an array of 16 electrodes located equidistant in a layer around the inside of the vessel. As fluids flow past the measurement plane, conductivity is measured in the 2D plane. The information on the state of the reaction and the fluid mixing can be extracted from the ERT measurements. Our ERT system can collect more than 100 datasets per second with 104 data points per dataset. Multiple test cases over a range of vessels, volumes, and chemical concentrations have been done. From 0.05 M to 4 M HCl and H2SO4 titrated with 0.1 M to 5 M NaOH. These reactions have an extensive conductivity range and provides the best case for identifying the reaction's endpoint and the extend of mixing in the test vessels. When compared to other methods to find the endpoint of the reaction, it can be seen that the data matches up closely with the other methods. Additionally, more accurate time points can be obtained by the online ERT system comparing to other methods. Another significant benefit of this ERT system is the ability to monitor the fluid mixing. This technology can be potentially used in reactors where visibility, testing access, or conditions restrict access to the vessel.

4:00 PM Using Molecular Dynamics to Study Separation Mechanisms of Monoatomic Gases Via DD3R Zeolite Membrane (WeD1b)

Bandar Bashmmakh (Illinois Institute of Technology), *Xiaoyu Wang* (University of Notre Dame), *Cynthia J. Jameson* (University of Illinois Chicago), *Sohail Murad* (Illinois Institute of Technology)

Noble gas fission byproducts, such as Kr and Xe, are generated within nuclear power reactors are currently being discharged into the atmosphere. This practice has a major economic drawback because of the high value associated with some of these gases. Separation of such gases has a high economical toll because of the high energy requirement associated with cryogenic distillation, the traditional process for such separations. Zeolites, nanoporous materials suitable for gas separation processes, have become of major interest due to the potentially high selectivity for such separations. We have used nonequilibrium molecular dynamics to investigate the separation performance of DD3R framework zeolitic membranes (using LAMMPS software package) for such separations. Our studies have shown that the DD3R membrane shows promise for high selectivity ratios of Kr over Xe. The effects of pressure, temperature and pure vs. mixture gas feed conditions are studied in this work to understand and explain, at the molecular level, the mechanisms of these (Kr/Xe) separations. MD runs show agreement with experimental trends of the permeation of Kr/Xe pure and mixed gases using DD3R zeolite with high separation factor. Despite the absence of Xe complete permeation through the membrane because of MD timescale limitations, our results are sufficient to describe the separation mechanisms including the much slower diffusion, caused by barrier-height-limited permeation, for Xe in comparison to Kr which is a desired trend in looking for high separation factors.

4:20 PM Foam Film Drainage of Milk Protein Derivative Nacas Vs Micellar Surfactant SDS (WeD1c)

Lena Hassan (University of Illinois Chicago), *Chenxian Xu* (University of Illinois Chicago), *Vivek Sharma* (University of Illinois Chicago)

Proteins in food, cosmetic and pharmaceutical foams influence the interfacial and bulk properties of formulations. In this study, we characterize the drainage of protein-based foams as well as single foam films, and contrast their behavior with micellar foams formed with small molecular surfactants above the critical micelle concentration. Micellar foam films undergo drainage via stratification manifested as step-wise thinning in the plots of average film thickness over time. Stratification in micellar foam films is accompanied by formation of coexisting thick-thin regions visualized in reflected light microscopy as exhibiting distinct grey regions as intensity is correlated with thin film interference. We critically examine the drainage of protein foam films to determine how and when stratification can be observed, and evaluate the connection between drainage of single foam films and bulk foams. We find that unlike flat domains in micellar SDS solutions with a sharp and circular moving front, and non-flat features we identify as nanoridges and mesas, the micellar NaCas solutions display non-flat domains, that grow by creating non-circular, finger-like patterns.

4:40 PM Rheology and Texture of Animal and Plant-Based Mayo Emulsions (WeD1d)

Nadia Nikolova (University of Illinois Chicago), *Lena Hassan* (University of Illinois Chicago), *Vivek Sharma* (University of Illinois Chicago)

Mayonnaise is an emulsion used as a dressing, a dip, and a base for sauces. The conventional recipe of mayo uses egg that influences the texture, taste, stability, and rheology of these animal protein-based concoctions. Often, mayo is presented as a challenging example of food materials made with animal-based proteins that are hard to emulate using plant-based proteins. In this contribution, we characterize the shear and extensional rheology response of animal and plant-based mayo emulsions, seeking to decipher the signatures that make real mayo into such an appetizing complex fluid.

<u>Energy Storage II</u>

Wednesday, March 2, 2022 (**<u>WeD2</u>**)
Chair: *Juan Garcia* (Argonne National Laboratory)
Co-Chair: *Hakim Iddir* (Argonne National Laboratory)

3:40 PM V2+/V3+ Reaction Intermediate By Surface Enhanced Raman Spectroscopy (WeD2a)

Daniel Pert (University of Michigan), *Bryan Goldsmith* (University of Michigan), *Harsh Agarwal* (University of Michigan), *Nirala Singh* (University of Michigan)

Vanadium redox flow batteries (VRFBs) are a promising technology for grid-scale energy storage of intermittent renewables such as wind and solar. However, their commercialization is limited due to poor V2+/V3+ electron-transfer kinetics and low power density. Understanding the V2+/V3+ charge-transfer mechanism by identifying the structure of the adsorbed reaction intermediate on electrodes can provide useful insights to design more effective electrolytes and electrocatalysts for V2+/V3+ reaction, improving performance of VRFBs. The V2+/V3+ reaction is previously hypothesized to go through an anion-bridged intermediate (i.e., V[(H2O)n(X)y]*, where X is a bridging anion), whose energy can be tuned to control the charge transfer. In this study, we aim to identify the structure of the V2+/V3+ intermediate on a polycrystalline Au surface in various electrolytes (e.g., HCl, HBr, HI, H2SO4) via surface-enhanced Raman spectroscopy (SERS) and ab initio density functional perturbation theory. To determine whether the proposed structure is accurate, we compare the Raman shifts obtained experimentally and computationally upon adsorption of the vanadium-ion complex on a metallic surface (e.g. from Au-OH to Au-O-V) with different anions (i.e., Cl-, Br-, I-, SO42-). Additionally, we show that the desorption barrier of this adsorbed V3+-ion complex can be used as a descriptor to explain charge transfer on metal electrodes, similar to glassy carbon reported previously.

4:00 Compressed Gas Energy Storage Integrated with Combined Heat and Power Plant (WeD2b)

Sebastiano Giardinella (University of Illinois Urbana-Champaign), *Alberto J. Baumeister* (Ecotek Engineering USA), *Richard Callahan* (Enerflex Inc), *Ramon Diaz* (Ecotek Investments Inc), *Daryl-Lynn Roberts* (Visage Energy Corp), *Kevin O'Brien* (University of Illinois Urbana-Champaign), *Leslie Gioja* (University of Illinois Urbana-Champaign), *Jim Dexter* (University of Illinois Urbana-Champaign), *Scott Prause* (University of Illinois Urbana-Champaign), *Ryan Larimore* (University of Illinois Urbana-Champaign), *Michael Larson* (University of Illinois Urbana-Champaign), *Robert Roman* (University of Illinois Urbana-Champaign), *Chinmoy Baroi* (University of Illinois Urbana-Champaign)

A new energy storage technology, Compressed Gas Energy Storage (CGES), seeks to achieve low-cost, long-duration energy storage by combining mature commercially-available technology (compressors, high-pressure gas storage, expander generators) and utilizing existing infrastructure for transportation and distribution of industrial gases (e.g., natural gas, hydrogen, oxygen, carbon dioxide, or others).

CGES utilizes existing compressors to transform electricity into potential energy (pressure), existing pipelines or underground storage to store said potential energy, and adds new expander generators at pressure reduction points in the network to recover part of the energy used in compression and transform it into electricity.

By adapting itself to widely available existing infrastructure, CGES recovers energy that is otherwise wasted in the gas value chain, reduces the cost of new facilities, and avoids many of the development hurdles typically associated with other long-duration energy storage technologies (e.g., Compressed Air Energy Storage, CAES).

This paper discusses the performance and economics associated with CGES as a standalone project and in combination with a thermal power plant, based on a concept for integration of the technology over an existing lateral pipeline transporting natural gas to an 85 MW combined heat and power plant that feeds power to a grid with increasing share of renewable power generation.

4:20 PM Active Learning for the Design of Naturally Occurring Organic Redox-Active Materials for Non-Aqueous Redox Flow Batteries (WeD2c)

Akash Jain (Argonne National Laboratory), *Rajeev Assary* (Argonne National Laboratory)

Non-aqueous redox flow batteries (NRFBs) are promising systems for grid-scale energy storage applications. However, the limited power and energy densities and the lack of suitable redox-active materials: catholyte, and anolyte in the electrolyte solution, limit the adoption of NRFBs at a large scale. To achieve higher power and energy densities in NRFBs, catholyte, and anolyte must display a large redox potential window and high solubility in the electrolyte solution. In this work, we investigate the suitability of inexpensive organic flavonoid molecules for NRFB catholyte and anolyte applications. Specifically, we study naturally occurring organic flavonoid molecules as scaffolds and decorate them with functional groups to modify their properties and generate about one million new flavonoid molecules. To accelerate the design and discovery of new catholyte and anolyte molecules that display both high redox potential window and high solubility, we employ the active learning (multi-objective Bayesian optimization) method to identify suitable molecules from a library of about one million molecules while using a small number of computationally expensive density functional theory (DFT) calculations. Overall, our work shows that naturally occurring organic flavonoid molecules are promising redox-active materials for NRFBs and with a multi-objective Bayesian optimization method we can design new materials that exhibit multiple desired properties.

4:40 PM Development of Eco-Friendly Phase Change Material for Low Temperature Energy Storage Applications (WeD2d)

Kamal Nayan (Rajiv Gandhi Institute of Petroleum Technology)

The increasing need for energy, along with growing environmental concerns, has accelerated the development of renewable energy sources, particularly materials for energy storage. The use of PCM (phase change materials) for TES (thermal energy storage) has recently emerged as one of the most promising areas of research. The researcher in this study has developed a novel eutectic mixture using bee wax and stearic acid. Paraffin has been the most investigated substance for TES applications because of its favorable chemical and thermophysical characteristics. However, because of rising environmental concerns and depleting crude reserves, there has been a strong call for researchers to investigate alternatives to paraffin wax. Authors in this investigation have looked upon various alternatives of paraffin and found bee wax to be the best alternative to paraffin because of its bio-origin and similar chemical and thermophysical properties. The selected material has a high latent heat of fusion (LHF), a suitable melting point (MT), is chemically stable, non-toxic, and is inexpensive and widely accessible. The bio-based origins of both fatty acid and bee wax ensure that the created substance is readily available and environmentally friendly. From differential scanning calorimetry, it has been found that the developed eutectic mixture has sufficient LHF and congruent MT. Thermal cycle testing validated its thermal stability up to 300 thermal cycles. And the developed eutectic mixture can be used as PCM for a variety of TES applications. Economic analysis has shown that our developed PCM for TES is cheap and readily available in the market.

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- **Catalysis & Reaction Engineering I and II**
  - Chair: *Trevor Lardinois* (Exponent)
  - Co-Chair: *Belma Demirel* (bp)
- **Fluid Dynamics, Fluid Properties, & Transport Phenomena**
  - Chair: *Robert Tsai* (Honeywell UOP)
  - Co-Chair: *Karthika Suresh* (University of Illinois Chicago)
- **Climate Solution: Action I and II**
  - Chair: *Dennis O’Brien* (Advisian)
- **Energy Storage I**
  - Chair: *Hakim Iddir* (Argonne National Laboratory)
  - Co-Chair: *Juan Garcia* (Argonne National Laboratory)
- **Energy Storage II**
  - Chair: *Juan Garcia* (Argonne National Laboratory)
  - Co-Chair: *Hakim Iddir* (Argonne National Laboratory)
- **Poster Session**
  - Chair: *Karthika Suresh* (University of Illinois Chicago)
  - Co-Chair *Daniel Christiansen* (University of Illinois Chicago)

High School Outreach Program

The American Institute of Chemical Engineers (AIChE) is proud to host Engineering Career Day for local high school students in concurrent to the AIChE 14th Annual Midwest Regional Conference. This event is a great opportunity for students to explore the exciting profession of a chemical engineer as well as other engineering disciplines. In partnership with Illinois Institute of Technology and University of Illinois at Chicago, this high school outreach program will be hosted virtually with interactive sessions including engineering expos, lab tours, networking with the professionals, and Q&A with the engineering panel! We invite you to discover the world of engineering with us, be inquisitive, and of course, have fun along the way!

If you have any questions, please contact the AIChE High School Outreach Committee at aiche.outreach.chicago@gmail.com.

Event Schedule

8:30 am	**Welcome Session**
8:50 am	**Engineering Expo** Meet current engineering students and learn about engineering clubs!
9:50 am	**10 Minute Break**
10:00 am	**Keynote Speaker – Kimberly D. Moore** *Founder and President, KDM Engineering*
11:00 am	**30 Minute Lunch Break**
11:30 am	**Engineering Panel** Learn about the day-to-day activities of practicing engineers and engineering students. Time to ask your most burning questions.
12:30 pm	**Networking with the Professionals** Join us for three 20-minute networking sessions and learn about engineering from practicing engineers.
1:50 pm	**10 Minute Break**
2:00 pm	**Lab Tours** Learn about the tools and equipment engineers use to change the world!
3:00 pm	**Closing Remarks**

HS Outreach Organizing Committee Chairs: Donald Chmielewski (IIT), Linh Quach (bp)

Keynote: 10:00 AM Tuesday, March 1, 2022

Growing up, Kimberly Moore was always good at math and science, but didn't know about engineering until she got to college. Now, as president of an engineering consulting firm that specializes in utilities, Moore is passionate about bringing women and minorities into the industry and letting them know there are options available to them in the field.

Check out https://hopin.com/events/aiche-engineering-career-day-2022 for more information about the event or email us at aiche.outreach.chicago@gmail.com.

Calling All Professional Engineers!

The American Institute of Chemical Engineers (AIChE) is hosting Engineering Career Day for Chicago local high school students to explore a career in engineering. As part of the event, we have a Networking with the Professionals session where high school students have an opportunity to learn more about engineering and ask questions in a small interactive group setting. Each group of high school students will be paired with one professional engineer and one university engineering student to discuss a career in engineering. Please be prepared to share about your career path and what you love about engineering! If you are interested in participating in the Networking with the Professionals, please fill out this form to express your interest. If you have any questions, please contact us at aiche.outreach.chicago@gmail.com.

MRC 2023

15th Annual AIChE Midwest Regional Conference

Chicago - Spring 2023

For programming and volunteer opportunities please contact the AIChE Chicago Section at aichechicago@gmail.com