



Artie McFerrin Department of
CHEMICAL ENGINEERING
TEXAS A&M UNIVERSITY

ChEGSA
TEXAS A&M UNIVERSITY

Chemical Engineering Graduate Student Association

presents

11th ANNUAL RESEARCH SYMPOSIUM

2024



Memorial Student Center



07th March 2024



07:15 AM to 05:00 PM

Welcome!!

We hope to highlight the research conducted in the Chemical Engineering Department of Texas A&M University through the 11th Annual ChEGSA symposium and provide students an opportunity to showcase their work to their peers and industry professionals. We gratefully appreciate the industrial and internal Texas A&M sponsors for their generous monetary and technical support. Our goal is to offer a forum for the discussion of ideas that will enhance science and technology. We hope the event is successful and productive for all attendees.

Meet the team!!

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Floor Plan - MSC

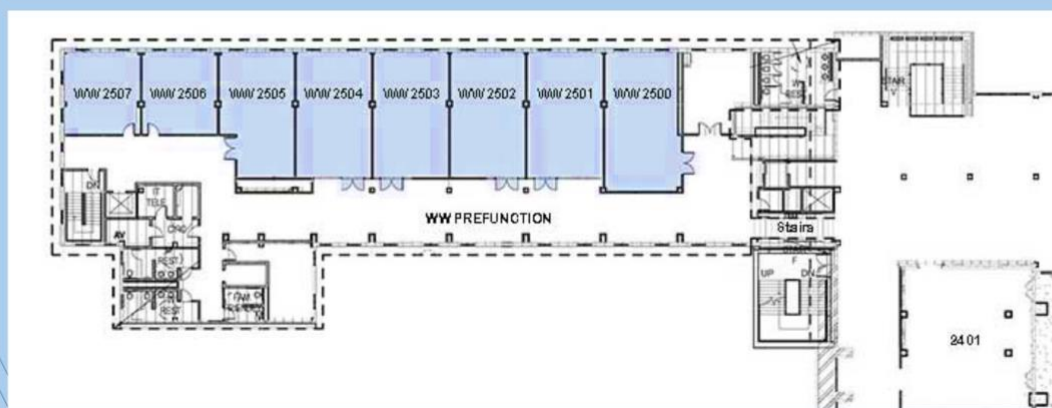


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Symposium Schedule

Thursday (7th March 2024), Memorial Student Center

Time	Event		
07:15 - 08:15	Registration (MSC 2400)		
	Breakfast (MSC 2400)		
08:15 - 08:25	Opening Remarks (MSC 2400)		
08:25 - 09:00	Keynote Address (MSC 2400)		
09:00 - 09:10	Transition/Coffee Break		
09:15 - 11:15	Oral Presentations		
	Advanced Materials and Nanotechnology (MSC 2501)	Health and Bioengineering (MSC 2502)	PSE and Data Science (MSC 2503)
	Transition		
	Plenary Talk (MSC 2406)		
11:20 - 11:55	Panel Discussion (MSC 2406)		
11:55 - 12:35	Lunch (MSC 2400)		
12:35 - 13:45	Guest Lecture: Chih-An Hwang (MSC 2406)		
13:45 - 14:30	TBD (MSC 2406)		
14:30 - 14:55	Transition/Coffee Break		
14:45 - 15:00	Poster & Networking Session (MSC 2400)		
15:00 - 16:30	Closing Remarks & Awards (MSC 2400)		
16:30 - 17:00			

Keynote Address



Dr. Mark Barteau

Professor,

Dept. of Chemical Engg. &

Dept. of Chemistry



08:25 AM - 09:00 AM



MSC 2400

Dr. Mark Barteau is a member of National Academy of Engineering; holder of the Halliburton Chair in Engineering and Professor in the Department of Chemical Engineering, College of Engineering and in the Department of Chemistry, College of Science. Prior to his joining at Texas A&M University, he was the Director of the University of Michigan Energy Institute at the University of Michigan, and the DTE Professor of Advanced Energy Research at the University of Michigan.

The importance of being a researcher

One of the classic reads for researchers is Sir Peter Medawar's "Advice to a Young Scientist" (1979). Despite having been written in another place and time, many of its observations are timeless and its commentaries remarkably prescient in their relevance to our time. As we researchers find ourselves buffeted by political winds and struggling with an apparent diminution of public confidence in science, it is worth revisiting the joys of discovery and the ongoing importance of our work to the human society of which we are a part.

Oral Presentations

Time	Advanced Materials and Nanotechnology (MSC 2501)	Health and Bioengineering (MSC 2502)	PSE and Data Science (MSC 2503)
09:15 - 09:30	Laxmi Sai Viswanadha	Harikrishnan Namboothiri	Natasha Jane Chrisandin
	<i>The influence of nanofillers and surface treatment on mechanical properties of ceramic nanocomposites</i>	<i>Modeling Recombinant Gene Expression Dynamics Across Bacterial Growth Phases</i>	<i>A Holistic Resilience Analysis for a Water-Energy Co-Generation Process</i>
09:30 - 09:45	David Kumar Yesudoss	Razeen Shaikh	Kenneth Kusima
	<i>Electrochemical Synthesis of Formamide from CO₂ and NH₃ using Titanium Nitride (Ti₂N) MXene</i>	<i>Optimal Performance Objectives in a Highly Conserved Cell-Cell Signaling System</i>	<i>A Machine Learned Enhancement to Transient Kinetic Models</i>
09:45 - 10:00	Bright Ngozichukwu	Assame Arnob	Jung Yoon (Timothy) Kim
	<i>Unprecedented Direct Methanol Coupling for Selective Conversion of CO₂ to Ethane</i>	<i>Influence of Physicochemical and Environmental Factors on Lipopolysaccharide Uptake by Synthetic Lipid Droplets</i>	<i>Recovering carbon losses in CO₂ electrolysis using a solid electrolyte reactor</i>
10:00 - 10:15	Siddhesh Borkar	Siddhant Gulati	Macro Pedro De Sousa
	<i>Using Strain as a Catalyst Design Tool to Enhance the Activity of Transition Metals and Climb Up the Volcano Plot</i>	<i>Complete enzymatic depolymerization of poly (ethylene terephthalate) (PET) plastic using a Saccharomyces cerevisiae-based whole-cell biocatalyst</i>	<i>Towards Real-time Carbon Emission Accounting and Scope Analysis to Optimize Hydrogen Production Decision Making</i>

Oral Presentations

Time	Advanced Materials and Nanotechnology (MSC 2501)	Health and Bioengineering (MSC 2502)	PSE and Data Science (MSC 2503)
10:15 - 10:30	Ray Yoo <i>Optimizing the Electrocatalytic Performance of Ti₂N MXene Through Decoupling Surface and Bulk Structure and Phenomena</i>	Bhavya Jaiswal <i>Bacteria Transformation using Microfluidic Continuous Electroporation in Paper (1/4CEP)</i>	Betsie Flores <i>A Systematic Multi-Scale Modeling and Optimization Framework for the Transition in Energy, Mobility, and Materials</i>
	Denis Johnson <i>Describing the Stable Mars-van Krevelen Catalytic Cycle for Green Ammonia Production on Nitride MXene</i>	Ting-Ching Wang <i>Genomic heterogeneity drives mechanical adaptation in human tumor cells.</i>	Ritu Ranjan <i>Fault-tolerant control with dynamic safety margin management in safety-critical system</i>
10:45 - 11:00	Omar El Arwadi <i>Time and Temperature-Dependent Fracture Mechanics of Self-Healing Vitrimers</i>		Marcello Di Martino <i>Food-Energy-Water Nexus Considerations in Modular Greenhouse Farming Optimization</i>
	Tanaya Mandal <i>Electrochemically Activated Ti₄N₃T_x MXene Electrodes for Batteries and Supercapacitors</i>		

Plenary Talk



Dr. Michael A. Reynolds
Senior Principal Science Expert
Shell Catalysts and Technologies



11:20 AM - 11:55 AM



MSC 2406

Michael A. Reynolds is the Senior Principal Science Expert for Shell Catalysts and Technologies, where he leads programs for catalyst development in conventional refining and projects for the energy transition. Since 2012, he has also served as an Adjunct Professor at Rice University in the Department of Chemical and Biomolecular Engineering (Houston, Texas). In this capacity he serves on student doctoral committees and provides lectures on special topics. Dr. Reynolds has developed catalysts for upgrading heavy oil into liquid fuels, for distillate hydroprocessing, and for hydroconversion of renewable feedstocks. Prior to his current role, Dr. Reynolds spent ten years in Shell's Shales business as a production chemist where he supported oilfield developments in west Texas, Canada, and Argentina for hydraulic fracturing and water treatment. His current research interests include renewable hydrocarbons, hydrogen, and applications of crystal engineering to new materials.

Crystal engineering approaches to water treatment

Acid-insoluble inorganic scales such as the sulfates of calcium, barium, and strontium are problematic contaminants that are commonly encountered in pipelines and water treatment facilities. These biominerals have low solubilities in water ($K_{sp} < 10^{-10}$) and are resistant to changes in pH, temperature, and flow conditions. In addition to these issues, naturally occurring radium-226 can co-crystallize within these scales leading to radioactive hazards. Most methods for remediation involve abrasive mechanical milling techniques that can damage equipment and increase maintenance costs for well or water processing operations. A more advantageous option would be to apply chemicals that can either inhibit scale formation, or dissolve scale that has already precipitated. Yet, few viable chemical options are commercially available. This presentation will focus on an approach to studying scale formation and remediation using the concept of a lab-on-a-chip. Recent results from laboratory studies of new chemical inhibitors and dissolvers based on green chemistry motifs will be introduced. A goal of this presentation is to introduce the scientific community to these challenges and to demonstrate the power of collaborative research with university partners.

Guest Lecture



Dr. Chih-An-Hwang

Senior Advisor (Retd.)

LyondellBasell Chemical



01:45 PM - 02:30 PM



MSC 2406

Dr. Chih-An Hwang, retired Senior Advisor at LyondellBasell Chemical, is renowned for his expertise in Advanced Process Control (APC) and polymer technologies. Notable contributions include optimizing Spheripol PP and Bayport C&E lines, leading Mega projects like Hyperzone HDPE and ADL/mPE startups, and spearheading APC initiatives at Chevron Phillips Chemical. With extensive experience in catalyst and process development, he holds multiple U.S. patents. As Chief Consultant at Pavilion Technologies, he pioneered Perfecter (NMPC) technology. His global impact encompasses consultancy for major polymer technologies worldwide. Formerly at Quantum Chemical, he played a pivotal role in APC consultancy and MPC development.

Non-linear Advanced Process Control in Industries

This presentation is about the pivotal role of Non-Linear Advanced Process Control (APC) in the Chemical Process Industries, with a focus on its application in polymer processing. Beginning with foundational aspects such as Control Systems Engineering (CSE), System Identification (SI), and essential APC Terminology, the discussion delves into the architecture of Non-Linear APC. Various Controller Design Methodologies, including Neural Network-based, first principles, and hybrid modeling, will be explored in detail. Rheology's significance in the context of processing and its correlation with Non-Linear APC will be elucidated. The presentation will then navigate through Polymer Non-Linear Model Predictive Control (NMPC) best practices, offering insights into its application. An examination of the gap between academia and industry in the realm of Advanced Control will be addressed, emphasizing the need for effective bridging. Drawing from extensive industrial experience, the presentation will provide practical perspectives on Non-Linear APC, culminating in a comprehensive conclusion.

Poster Presentations

Poster No.	Presenter	Presentation Title
P1	<i>Md. Saifur Rahman</i>	Engineered hydrogel-based microelectronics for recording and neuromodulation
P2	<i>Catherine Nkoutche</i>	Multi-Objective Mixed Integer Optimization Model for Proactive Planning Tool for an Integrated Strategic Framework in Resilience & Sustainability of Supply Chain Networks
P3	<i>David Kumar Yesudoss</i>	Electrochemical Synthesis of Formamide from CO ₂ and NH ₃ using Titanium Nitride (Ti ₂ N) MXene
P4	<i>Laura Hoagland</i>	Improving lithium-ion energy storage through novel 2D electrode materials
P5	<i>Somtochukwu Lambert</i>	Radio frequency-driven catalytic dehydrogenation of propane for propylene production.
P6	<i>Siddhi Kotnis</i>	High-efficiency PET degradation with a two-enzyme system immobilized on Magnetic Nanoparticles
P7	<i>Sahithi Srijana Akundi</i>	Risk-based Model Predictive Controller via Chance-Constrained programming
P8	<i>Jitendra Choudhary</i>	Large-scale Assemblies of TiC Nanowires for High-Temperature Applications
P9	<i>Amani Grati</i>	Evaluation of the maximum gas generation rate under runaway conditions: Comparative analysis of the available methodologies
P10	<i>Harikrishnan R Namboothiri</i>	Modeling Recombinant Gene Expression Across Bacterial Growth Stages