

**ChEGSA**  
TEXAS A&M UNIVERSITY

**Chemical Engineering Graduate Student Association**

# **6<sup>th</sup> Annual Research Symposium**

**Friday, March 8th, 2019  
8:00 am - 4:00 pm  
MSC, TAMU**



## TABLE OF CONTENTS

<b>Sponsors .....</b>	<b>2</b>
<b>Welcome .....</b>	<b>3</b>
<b>Schedule .....</b>	<b>4</b>
<b>Exhibitors .....</b>	<b>5</b>
<b>Keynote Address.....</b>	<b>6</b>
<b>Oral Presentations - Morning Session.....</b>	<b>7</b>
<b>Oral Presentations - Afternoon Session.....</b>	<b>8</b>
<b>Poster Session .....</b>	<b>9</b>
<b>Building Layout .....</b>	<b>15</b>

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TEXAS A&M ENERGY INSTITUTE

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## WELCOME

On behalf of the organizing committee we extend you a warm welcome to College Station and the 6th Annual Research Symposium. The purpose of the symposium is to showcase the research conducted in the department and provide students with an opportunity to present their research to industrial representatives. We gratefully acknowledge the sponsorship provided by Ascend Performance Materials, The Dow Chemical Company, Shell, NETZSCH, BASF, The Association of Former Students, Texas A&M Energy Institute, and Mary Kay O'Connor Process Safety Center. This symposium represents the ideal environment for the exchange of ideas to aid in the advancement of science and technology. We wish all the participants a productive and enjoyable event.

### ADVISORY COMMITTEE

<b>Dr. Arul Jayaraman</b>	<b>Dr. Perla Balbuena</b>	<b>Dr. Jodie Lutkenhaus</b>	<b>Dr. Katy Kao</b>
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### ORGANIZING COMMITTEE

<b>Hallie Graham</b>	<b>Harold Escobar</b>	<b>Yifei Yang</b>
<b>Mahesh Agrawal</b>	<b>M. Stefany Angarita</b>	<b>Rachit Gupta</b>
<b>Joseph Jakubowski</b>	<b>Kathy Rhee</b>	<b>Michael Bae</b>
<b>Naveen K. Mishra</b>	<b>Nutan Patil</b>	<b>Jacob Gruener</b>
<b>Ashwini Ravindran</b>	<b>Edwin Lavi</b>	<b>Opeyemi Olojede</b>
<b>Dongheon Lee</b>	<b>Rushant Sabnis</b>	

### CONTACT US

**EMAIL:** [chegsa@chegsa.tamu.edu](mailto:chegsa@chegsa.tamu.edu)

**WEBSITE:** <https://www.chegsatamu.com/>

**LINKEDIN:** Texas A&M Chemical Engineering Graduate Student Association (ChEGSA)

# SCHEDULE

TIME	EVENT			
8:00 A.M. - 8:45 A.M.	Breakfast and Registration - 2401			
8:45 - 9:00	Opening Remarks - 2400			
9:00 - 9:30	Keynote Address - 2400			
9:30 - 9:40	Transition			
	<b>Advanced Materials &amp; Bioengineering</b>	<b>Energy</b>	<b>Process Engineering &amp; Optimization</b>	<b>Process Safety</b>
	<b>Track A - 2500</b>	<b>Track B - 2502</b>	<b>Track C - 2504</b>	<b>Track D - 2402</b>
9:40 - 10:00	Ethan Kamphaus	Manali Zantye	Baris Burnak	Denis Su F.
10:00 - 10:20	Nutan Patil	William Tso	Burcu Beykal	Cassio Brunoro A.
10:20 - 10:40	Tzu L. Chen	Chi Zhang	Abhinav Narasingam	Jingyao Wang
10:40 - 11:00	Transition			
11:00 - 12:00	Networking Session - 2400			
12:00 - 1:00	Lunch - 2400			
1:00 - 2:00	Poster Session - 2406 A			
2:00 - 2:20	Transition			
2:20 - 2:40	Kathy Rhee	Akhil Arora	Salih E. Demirel	Nilesh Ade
2:40 - 3:00	Akshi Singla	Prashanth K. Siddhamshetty	Mohammed S. F. Bangi	Andreas Ehnbonm
3:00 - 3:30	Break			
3:30 P.M. - 4:00 P.M.	Closing Remarks and Awards - 2400			

<b>Energy</b>	<b>Advanced Materials</b>	<b>Bioengineering</b>	<b>Process Engineering and Optimization</b>	<b>Process Safety</b>
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## **EXHIBITORS**

**MSC2400**

**All the booths will be located in ballroom, come see our exhibitors during the networking hour and breaks in MSC 2400!**

<b>Booth Number</b>	<b>Exhibitors</b>
<b>1</b>	<b>ASCEND</b>
<b>2</b>	<b>BASF</b>
<b>3</b>	<b>DOW</b>
<b>4</b>	<b>NETZSCH</b>

## KEYNOTE ADDRESS - Dr. Vikram Gopal



**Vikram Gopal, Ph.D.**

Sr. Vice President Technology,  
Ascend Performance Materials, Houston, Texas, USA

### **The One Constant: Embracing Change in the Chemical Industry**

Vikram Gopal has broad experience in the advanced materials industry with expertise in research and development, product development, process engineering and applications development. Before joining Ascend Performance Materials in May 2015, he was vice president of technology at Invista Engineering Polymer Solutions. Vikram has vast knowledge of the nylon 6,6 market and is credentialed as a Six Sigma Black Belt.

Vikram has been recognized for multiple industry awards for rapid product development and value creation for his teams. He holds a bachelor's degree in petrochemical engineering from the University of Pune in India, a doctorate degree in chemical engineering from the University of Alabama and an MBA from the University of Michigan's Ross School of Business.



## ORAL PRESENTATIONS – Morning Session

Time	Advanced Materials & Bioengineering	Energy	Process Engineering & Optimization	Process Safety
	Track A MSC 2500	Track B MSC 2502	Track C MSC 2504	Track D MSC 2405
9:40 -10:00	<b>Li Dendrite Nucleation from First Principles Perspective</b>  <i>Ethan Kamphaus</i>	<b>Dynamic Power Plant Scheduling with Flexible Carbon Capture in Uncertain Electricity Markets</b>  <i>Manali Zantye</i>	<b>A Multiparametric Programming Based Approach to Integrate Design, Scheduling, and Control of a Batch Process</b>  <i>Baris Burnak</i>	<b>Simultaneous Design and Control of an Inherently Safer Extractive Distillation Column</b>  <i>Denis Su F.</i>
10:00-10:20	<b>Radio Frequency Processing of Pre ceramic Polymer Nanocomposites and its Application.</b>  <i>Nutan Patil</i>	<b>Toward Supply Chain Optimization of Renewable Energy Carriers</b>  <i>William Tso</i>	<b>Data-Driven Optimization with Implicit Constraints: Application to an Ethane Steam Cracking Process</b>  <i>Burcu Beykal</i>	<b>Effects of Obstacle Configuration on Flame Propagation Regimes and Explosion Severity</b>  <i>Cassio Brunoro A.</i>
10:20-10:40	<b>Room Temperature Solid-State Lithium Polymer Battery with Polyionic Liquid Pentablock Terpolymer Electrolyte</b>  <i>Tzu L. Chen</i>	<b>Reliability Analysis in Synthesis of Direct Water Recycle Networks</b>  <i>Chi Zhang</i>	<b>Data-Driven Identification of Interpretable Reduced-Order Models Using Sparse Regression</b>  <i>Abhinav Narasingam</i>	<b>Experimental Study of Electrostatic Hazard inside Scrubber Column Using Response Surface Methodology</b>  <i>Jingyao Wang</i>



## ORAL PRESENTATIONS – Afternoon Session

Time	Advanced Materials & Bioengineering	Energy	Process Engineering & Optimization	Process Safety
	Track A MSC 2500	Track B MSC 2502	Track C MSC 2504	Track D MSC 2405
2:20-2:40	<b>Flagellar Hydrodynamics in <i>Bacillus subtilis</i></b>  <i>Kathy Rhee</i>	<b>Dynamically-Intensified Adsorption-Reaction Processes for Unconventional Natural Gas Utilization</b>  <i>Akhil Arora</i>	<b>Building Block-Based Design and Intensification of Chemical Processes</b>  <i>Salih E. Demirel</i>	<b>Safer design and operation of Proton Exchange Membrane Fuel Cells</b>  <i>Nilesh Ade</i>
2:40-3:00	<b>Novel Technique to Target Bacteria, <i>Pseudomonas Aeruginosa</i>, via Hetero-Multivalent Binding</b>  <i>Akshi Singla</i>	<b>Modeling and Control of Proppant Distribution of Multi-Stage Hydraulic Fracturing in Horizontal Wells</b>  <i>Prashanth K. Siddhamshetty</i>	<b>Enlarging the Domain of Attraction of Local Dynamic Mode Decomposition with Control Technique: Application to Hydraulic Fracturing</b>  <i>Mohammed S. F. Bangi</i>	<b>Homeomorphic Isomerism in Macrobicycles</b>  <i>Andreas Ehnborn</i>

# POSTER SESSION

MSC 2406A

01:00 P.M. – 02:00 P.M.

Poster Number	Name of Presenter	Poster Title
1	Yuchan Ahn	Development of the Optimization Model for the Shale Gas Production with Water Management Considering the Control of Hydraulic Fracturing System in the Unconventional Wells
2	Hyun K. Choi	Designing a Model-Based Feedback Control Framework of Kappa Number and Porosity with a Multiscale Modeling
3	Dongheon Lee	Construction of a Semi-Stochastic Intracellular Signaling Model Via Global Sensitivity Analysis and Probability Density Estimation
4	Jianping Li	Process Innovation Using Block Superstructure
5	Naveen Mishra	Multilayer Polymeric Films on Hollow Fibers for Light Gas Separation
6	Kasturi Sarang	Tannic Acid as a Small Molecule Binder for Silicon Anodes in Lithium-Ion Batteries
7	C. Doga Demirhan	An Integrated Data-Driven Modeling & Global Optimization Approach for Production Planning
8	Xiaofei Zhao	Anti-oxidants unlock shelf-stable Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> (MXene) nanosheet dispersion
9	Spyridon Tsolas	Systematic Analysis, Design and Optimization of Water-Energy Nexus
10	Dali Huang	Magnetically Driven Functionalized Nanoplatelets Pickering Emulsion for Removal of Oil Contaminants from Water
11	Rachit Gupta	Engineering Design and Optimization of Protein Transformation into Bacterial Cells
12	Yuhe Tian	Towards the Incorporation of Operability and Safety in the Synthesis of Intensified Reactive and Extractive Separation Systems

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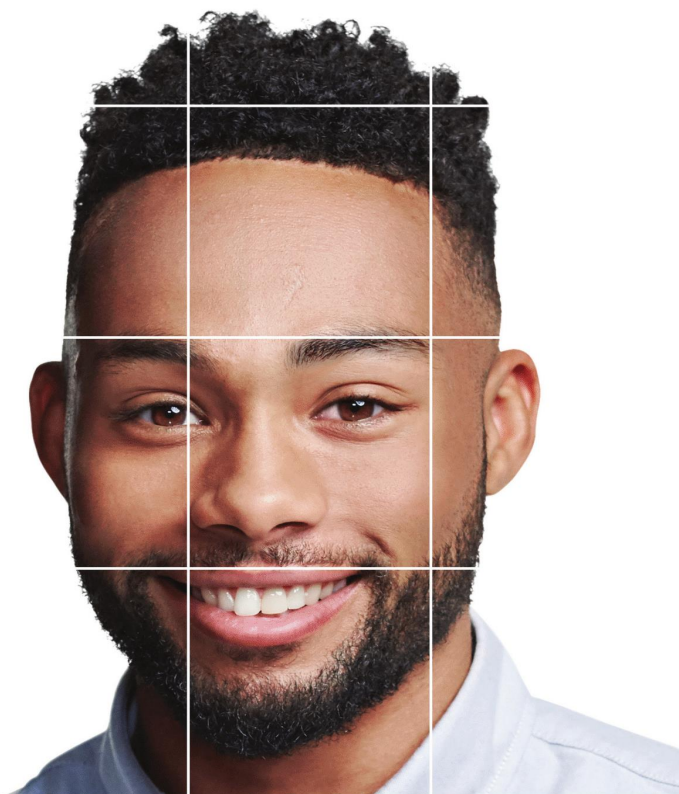
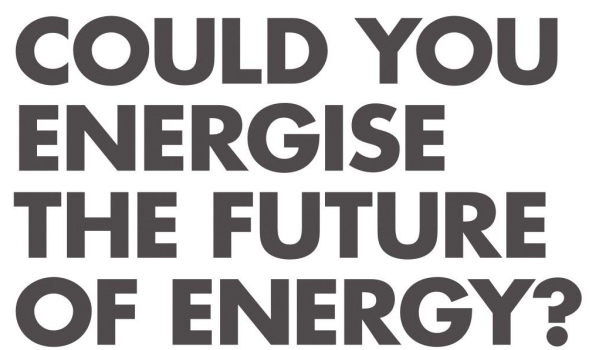
Through our employee-led foundation our people contribute time and money to local causes. We focus on education, hunger, housing, military support and children's health.

If you're ready to grow, learn, develop, contribute and give back, we'll be on campus for recruiting. We're looking for engineering co-ops, interns and employees ready for an opportunity.

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## Chemical Engineering Graduate Student Association



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The Texas A&M Energy Institute engages undergraduate and graduate students, postdoctoral associates, research staff, and faculty members toward the study and development of innovative technologies and policies for energy production and energy conservation. Special attention is paid to elucidating the complexity among the interacting components of energy, economics, law, public policy, and the environment. With 270 faculty affiliates from nine colleges and schools, more than 20 Texas A&M University departments, two Texas A&M University branch campuses, and two Texas A&M University System member institutions, along with a unique community of more than 450 doctoral students and postdoctoral fellows in the Texas A&M Energy Research Society, cutting-edge solutions are being realized through true interdisciplinary collaborations that will address the complexity and challenges of the world's energy future.



energy.tamu.edu

Texas A&M Energy Institute | Frederick E. Giesecke Engineering Research Building  
3372 TAMU | College Station, TX 77843-3372 | energy.tamu.edu

In-Person/Online

Module-Based

10 Months

Thesis/Non-Thesis



## MAKING SAFETY SECOND NATURE

### ABOUT THE CENTER

The Mary Kay O'Connor Process Safety Center is the world's foremost university-based process safety center. The center serves industry, government, academia and the public, is a resource in education and research, & provides service to all stakeholders. Over the past 20 years, the body of work created by the center has led to its inarguable recognition as an unbiased science-based organization focused on creating dialogue and consensus on difficult scientific topics, amongst all stakeholders. The guidance of a steering committee of consortium member companies and a technical advisory committee of industry expert ensures that center activities are relevant to the actual practice of process safety.



### EDUCATION

Students pursuing doctoral degrees and master of science in safety engineering degrees under the auspices of the MKOPSC come from various fields of study, including chemical engineering, mechanical engineering, petroleum engineering and materials science and engineering.

#### ACADEMIC DEGREES AND CERTIFICATES

- Master of Science in Safety Engineering (also offered via distance learning)
- Safety Practice Certificate (for graduate and undergraduate students)

#### CONTINUING EDUCATION

- Safety Practice Certificate (for professionals)
- Continuing Education Courses (on site for professionals, 55 courses available)

#### INTERNSHIPS AND PLACEMENT

- ABS Consulting
- BakerRisk
- BASF
- Bayer
- BP
- DNV
- ExxonMobil Corp.
- Huntsman
- KBR
- Mustang
- Shell Oil Co.
- Siemens

**TEES**  
**MARY KAY O'CONNOR**  
**PROCESS SAFETY CENTER**  
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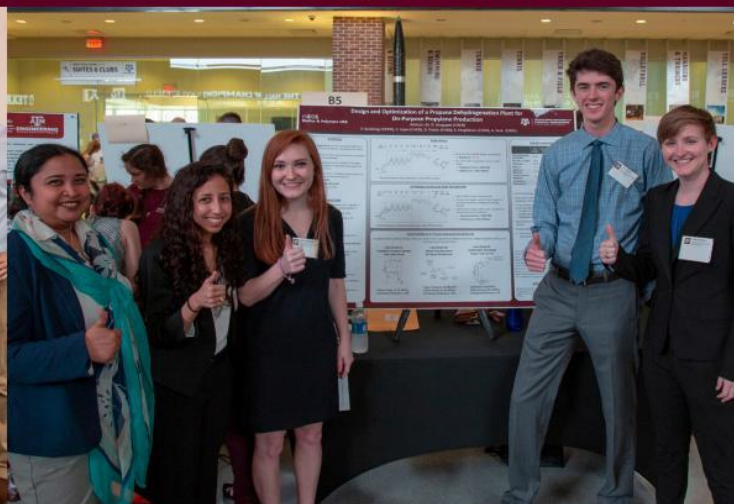




# ARTIE MCFERRIN DEPARTMENT OF CHEMICAL ENGINEERING

TEXAS A&M UNIVERSITY

## 2018 Department Fact Sheet



The Artie McFerrin Department of Chemical Engineering is one of the top rated chemical engineering departments in the world. In 2018, *U.S. News and World Report* ranked the undergraduate and graduate programs 13 and 12 respectively. It is also one of the largest, fully accredited chemical engineering programs in the country. The department has become a prolific chemical engineering research hub, with the faculty producing more than 240 refereed journal publications in 2018.

Located in the 205,000 square-foot, Jack E. Brown Chemical Engineering Building, the department provides its students and faculty members access to the latest resources, including 88 research and teaching facilities, six general classrooms, 13 conference rooms, and four computer laboratories.

## Research

The Artie McFerrin Department of Chemical Engineering at Texas A&M University has faculty engaged in a wide breadth of studies ranging from highly applied research in the areas of biomass utilization, process safety and hydrocarbon processing to very fundamental research in nanotechnology, life sciences, process systems engineering and molecular simulation. The ultimate goal of the research is to positively impact society by providing new knowledge.

## Department Research Areas

- Biomedicine | Biomolecules
- Biofuels | Biotechnology
- Catalysis and Reaction Engineering
- Complex Fluids | Microfluidics | Soft Matter
- Computational Chemical Engineering
- Energy
- Environmental | Sustainability
- Materials | Microelectronics
- Multiscale Systems Engineering
- Nanotechnology
- Process Control and Systems Engineering

## Department Head

**M.Nazmul Karim** | Professor | T. Michael O'Connor Chair II  
nazkarim@tamu.edu

## Enrollment

<b>Total Enrollment</b>	<b>1,066</b>
<b>Undergraduate</b>	<b>835</b>
<b>Graduate</b>	<b>231</b>
Master's	85
Ph.D.	146

## Faculty

<b>Total Faculty</b>	<b>40</b>
Professors	14
Endowed Chairs	5
Endowed Professorships	6
Endowed Faculty Fellows	5
TEES Eminent Professors	3
Associate Professors	9
Assistant Professors	8
Lecturers/Senior Lecturers	7
Professors of Practice	2
Senior Professors	3
Referred Journal Publications	240

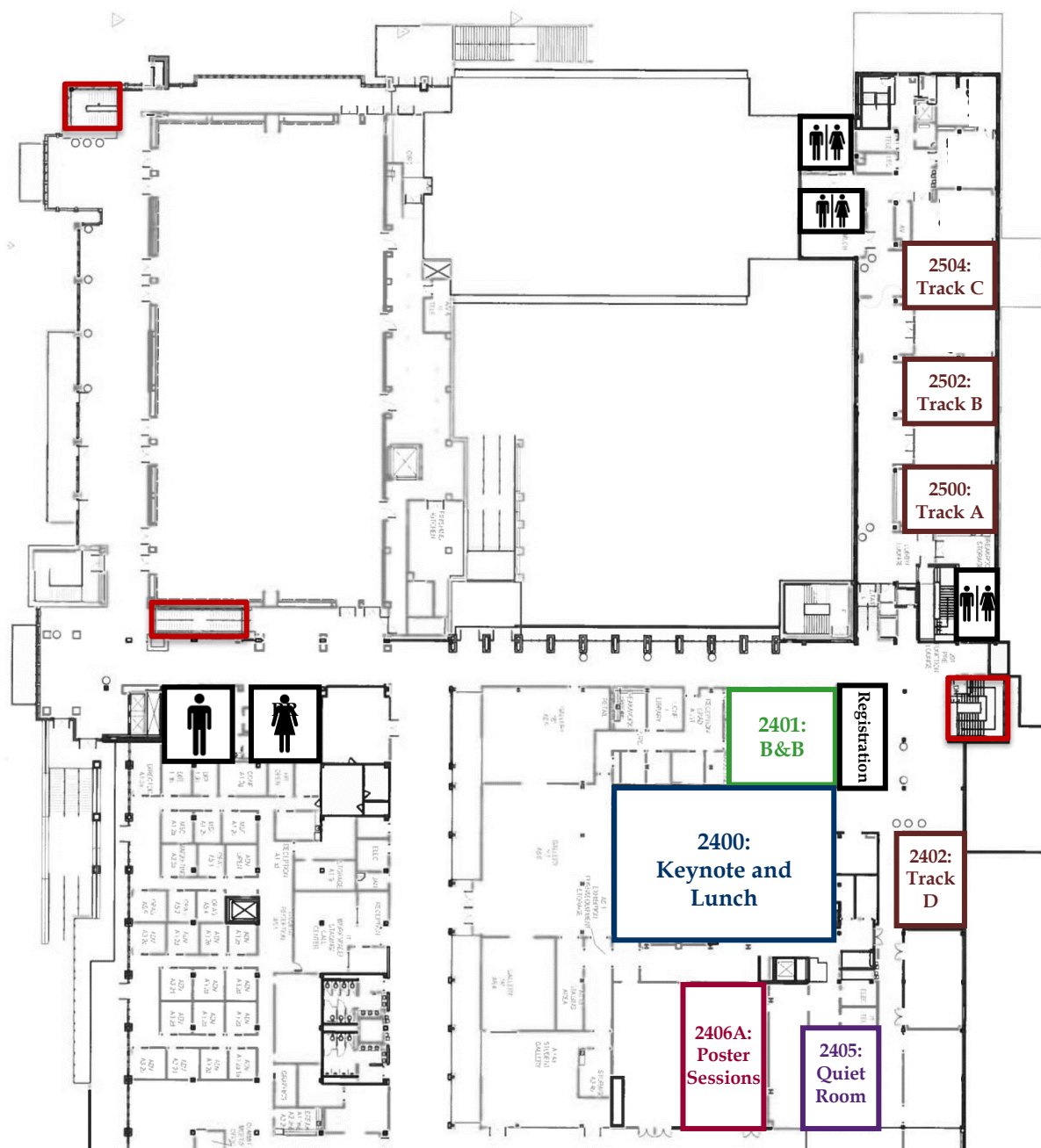
## Rankings

- #13** Undergraduate Program  
(*U.S. News & World Report*, 2018)
- #12** Graduate Program  
(*U.S. News & World Report*, 2018)

[engineering.tamu.edu/chemical](http://engineering.tamu.edu/chemical)



# BUILDING LAYOUT



Memorial Student Center (MSC) 2<sup>nd</sup> Floor

**2400: Keynote Address and**

**2401: Breakfast & Breaks (B&B)**

**2406A: Poster Sessions**

**2500: Track A: Advanced Materials & Bioengineering**

**2502: Track B: Energy**

**2504: Track C: Process Engineering & Optimization**

**2402: Track D: Process Safety**

**2405: Quiet Room**

**Emergency Exits Marked**

5<sup>th</sup> Chemical Engineering Graduate Student Association  
**ANNUAL RESEARCH SYMPOSIUM**

Friday, March 9, 2018 | 8:00 am - 3:30 pm | MSC, Texas A&M University



TABLE OF CONTENTS

Sponsors.....2

Welcome .....3

Schedule.....4

Keynote Address .....5

Oral Presentations – Morning Session .....6

Oral Presentations – Afternoon Session.....7

Poster Session I.....8

Poster Session II ..... 10

Building Layout.....16

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## WELCOME

On behalf of the organizing committee we extend you a warm welcome to College Station and the 5<sup>th</sup> Annual Research Symposium. The purpose of the symposium is to showcase the research conducted in the department and provide students with an opportunity to present their research to industrial representatives. We gratefully acknowledge the sponsorship provided by Eastman Chemical Company, Shell, The Association of Former Students, The Dow Chemical Company, and The Kaneka Foundation; also, the donations from BASF and the Texas A&M Student Engineering Council. This symposium represents the ideal environment for the exchange of ideas to aid in the advancement of science and technology. We wish all the participants a productive and enjoyable event.

## ADVISORY COMMITTEE

**Dr. Arul  
Jayaraman**

**Dr. Perla  
Balbuena**

**Dr. Jodie  
Lutkenhaus**

**Dr. Katy  
Kao**

## ORGANIZING COMMITTEE

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**Pranav Bagaria**

**Hallie Graham**

**Cassio Brunoro  
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**LINKEDIN:** [Texas A&M Chemical Engineering Graduate Student Association \(ChEGSA\)](#)

# SCHEDULE

Time	Event			
8:00 – 8:45	Breakfast and Registration (MSC 2401)			
8:45 – 9:00	Opening Remarks (MSC 2400)			
9:00 – 9:30	Keynote Address by Dr. Scott Armentrout (MSC 2400)			
9:30 – 9:40	Transition			
	<b>Track A- MSC 2500</b> <i>Advanced Materials</i>	<b>Track B- MSC 2502</b> <i>Bioengineering and Polymers</i>	<b>Track C- MSC 2504</b> <i>Process Systems Engineering</i>	<b>Track D- MSC 2405</b> <i>Computational Modeling and Process Safety</i>
9:40 – 10:00	● Febrian Hillman	● Michelle L. Olson	● Burcu Beykal	● Behnaz Rahmani
10:00 – 10:20	● L. Eric Zhang	● Jyot Antani	● Baris Burnak	● Pritishma Lakhe
10:20 – 10:40	● Tianyu Kelvin Yuan	● Dongheon Lee	● Jianping Li	● C. Doga Demirhan
10:40 – 10:50	Break (MSC 2401)			
10:50 – 11:50	Poster Session I (MSC 2300A)			
11:50 – 1:00	Lunch and Networking (MSC 2400)			
1:00 – 2:00	Poster Session II (MSC 2300A)			
2:00 – 2:10	Break (MSC 2401)			
2:10 – 2:30	● Hyosung An	● Yi-Yun Timothy Tsao	● Eric Bohac	● Ankita Taneja
2:30 – 2:50	● Smit A. Shah	● Pilar Suarez-Martinez	● Justin Katz	● Srikanth Panyaram
2:50 – 3:10	● Glenn Zeng	● Yanpu Zhang	● Spyridon D. Tsolas	● Ashwin Agarwal
3:10 – 3:20	Transition			
3:20 – 3:30	Closing Remarks and Awards (MSC 2400)			

<b>Research Focus</b>	● Advanced Materials	● Bioengineering	● Process Safety
	● Process Systems Engineering	● Polymers	● Computational Modeling

## KEYNOTE ADDRESS - Dr. Scott Armentrout



**Scott Armentrout, Ph.D.**  
**Director, External Innovation, Eastman Chemical Company**

### **Innovation in the Chemical Industry: Enhancing the Quality of Life in a Material Way**

Scott Armentrout is the Director of External Innovation for Eastman Chemical Company. Armentrout has responsibility for the identification and coordination of collaborative growth initiatives between various academic and industrial agencies and Eastman. Armentrout was previously Manager, Applications Innovation for Eastman Chemical Company. In that position, he had leadership responsibilities for the establishment of an interdisciplinary technology organization within Corporate Innovation to identify new growth opportunities for Eastman.

Armentrout joined Eastman in 1999 as a synthetic polymer chemist. Throughout his career, he has held several technology and people leadership positions of increasing level of responsibility across multiple technology and market platforms including polyester product and process development, cellulose ester product development, electronic chemicals innovation, and front end innovation.



## ORAL PRESENTATIONS – Morning Session

Time	Track A MSC 2500 <i>Advanced Materials</i>	Track B MSC 2502 <i>Bioengineering and Polymers</i>	Track C MSC 2504 <i>Process Systems Engineering</i>	Track D MSC 2405 <i>Computational Modeling and Process Safety</i>
9:40 – 10:00	<b>Rapid One-Pot Microwave Synthesis of Mixed Linker Hybrid Zeolitic-Imidazolate Framework Membranes for Tunable Gas Separations</b>  <u>Febrian Hillman</u> , Jordan Brito, and Hae-Kwon Jeong	<b>Relative Abundance of <i>Candida Albicans</i> and <i>Candida Glabrata</i> in <i>in vitro</i> Co-culture Biofilms Impacts Biofilm Structure and Formation</b>  <u>Michelle L. Olson</u> , Arul Jayaraman, and Katy C. Kao	<b>Optimal Design of Energy Systems Using Constrained Grey-Box Multi-objective Optimization</b>  <u>Burcu Beykal</u> , Fani Boukouvala, Christodoulos A. Floudas, and Efstratios N. Pistikopoulos	<b>Adsorption of Carbon on Partially Oxidized Cu Surfaces - Applications to Graphene Synthesis</b>  <u>Behnaz Rahmani Didar</u> and Perla B. Balbuena
10:00 – 10:20	<b>Micro-encapsulation with Nanoplatelet Surfactant</b>  <u>L. Eric Zhang</u> and Zhengdong Cheng	<b>Modulation of Ultrasensitive Signaling in Bacteria by Viscous Load on Flagellar Motor</b>  <u>Jyot Antani</u> and Pushkar Lele	<b>Integration of Design, Scheduling, and Control of Combined Heat and Power Systems: A Multiparametric Programming Based Approach</b>  <u>Baris Burnak</u> , Justin Katz, Nikolaos A. Diangelakis, and Efstratios N. Pistikopoulos	<b>Calorimetric Study of Graphene Oxide Thermal Stability</b>  <u>Pritishma Lakhe</u> , Devon Kulhanek, Wanmei Sun, Bin Zhang, Micah J. Green, and M. Sam Mannan
10:20 – 10:40	<b>Multifunctional Charge Transfer-Based Supramolecular Materials with Tunable Thermochromism</b>  <u>Tianyu Kelvin Yuan</u> , Lei Fang, and Mark A. Olson	<b>Stochastic Modeling of CTB-GM1 Binding Kinetics</b>  <u>Dongheon Lee</u> , Alec Mohr, Joseph S. Kwon, and Hung-Jen Wu	<b>Simultaneous Process Network Synthesis and Process Intensification Using Block Superstructure</b>  <u>Jianping Li</u> , Salih Emre Demirel, and M. M. Faruque Hasan	<b>Toward Optimal Synthesis of Renewable Ammonia and Methanol Processes</b>  <u>C. Doga Demirhan</u> , William W. Tso, and Efstratios N. Pistikopoulos
10:40 – 10:50	Break (MSC 2401)			
10:50 – 11:50	Poster Session I (MSC 2300A)			
11:50 – 1:00	Lunch and Networking (MSC 2400)			
1:00 – 2:00	Poster Session II (MSC 2300A)			
2:00 – 2:10	Break (MSC 2401)			



## ORAL PRESENTATIONS – Afternoon Session

Time	Track A MSC 2500  <i>Advanced Materials</i>	Track B MSC 2502  <i>Bioengineering and Polymers</i>	Track C MSC 2504  <i>Process Systems Engineering</i>	Track D MSC 2405  <i>Computational Modeling and Process Safety</i>
2:10 – 2:30	<b>Surface-Agnoistic Highly Stretchable and Bendable Conductive MXene Multilayers</b>  <i>Hyosung An, Touseef Habib, Smit Shah, Huili Gao, Miladin Radovic, Micah J. Green, and Jodie L. Lutkenhaus</i>	<b>Synthetic, Functional Thymidine-Derived Polydeoxyribo-nucleotide Analogues from a Six-membered Cyclic Phosphoester</b>  <i>Yi-Yun Timothy Tsao, Travis H. Smith, and Karen L. Wooley</i>	<b>Shale Gas Techno-economic Analysis: Designing Separation Units to Handle Feedstock Variability</b>  <i>Eric Bohac, Mahmoud El-Halwagi, and Debalina Sengupta</i>	<b>Improved Flare Radiation Criteria in Terms of Solar Radiation Contribution</b>  <i>Ankita Taneja, Delphine Laboureur, Bin Zhang, and M. Sam Mannan</i>
2:30 – 2:50	<b>3D Graphene Oxide Gel Assembly: Effects of Nanosheet Morphology and Ammonia on Gel Properties and Their use as Structural Electrodes for Energy Storage</b>  <i>Smit A. Shah, Dorsa Parviz, Morgan G. Odom, Wanmei Sun, Devon Kulhanek, and Micah J. Green</i>	<b>Polymer-Clay Nanocomposite Coatings as Efficient, Environment-Friendly Surface Pretreatments for Aluminum Alloy 2024-T3</b>  <i>Pilar C. Suarez-Martinez, Jerome Robinson, Hyosung An, Robert C. Nahas, Douglas Cinoman, and Jodie L. Lutkenhaus</i>	<b>Model Approximation in Multiparametric Optimization and Control – A Computational Study</b>  <i>Justin Katz, Nikolaos A. Diangelakis, and Efstratios N. Pistikopoulos</i>	<b>Predicting Influence of Packing Shape and Loading Methodology upon Fixed-Bed Structures</b>  <i>Srikanth Panyaram and Benjamin Wilhite</i>
2:50 – 3:10	<b>High Efficient Oil-Water Separation using Surface-Programmable Membranes</b>  <i>Glenn Zeng, Lecheng Zhang, Dali Huang, and Zhengdong Cheng</i>	<b>Water and Ion Pairing Universally Influence the Glass Transition of Polyelectrolyte Complexes</b>  <i>Yanpu Zhang, Piotr Batys, Joshua T O’Neal, Fei Li, Maria Sammalkorpi, and Jodie L. Lutkenhaus</i>	<b>Systematic Analysis and Optimization of Water-Energy Nexus</b>  <i>Spyridon D. Tsolas, M. Nazmul Karim, and M. M. Faruque Hasan</i>	<b>A Sustainable Process Design Approach for On-purpose Propylene Production and Intensification</b>  <i>Ashwin Agarwal, Debalina Sengupta, and Mahmoud M. El-Halwagi</i>
3:10 – 3:20	<b>Transition</b>			
3:20 – 3:30	<b>Closing Remarks and Awards (MSC 2400)</b>			

## POSTER SESSION I

MSC 2300A

10:50 A.M. – 11:50 A.M.

### Advanced Materials

- P.1 Polymerized Ionic Liquid Triblock Terpolymers: Synthesis and Characterization**  
*Patrick M. Lathrop and Yossef A. Elabd*
- P.2 Aramid Nanofiber/Functionalized Graphene Composite Electrodes for Structural Energy and Power**  
*Paraskevi Flouda, Dimitris C. Lagoudas, and Jodie L. Lutkenhaus*
- P.3 Radio Frequency Curing of Preceramic Polymers Loaded with Nano-fillers to Silicon Carbide Preforms**  
*Nutan Patil, Micah J. Green and Mohammad Saed*
- P.4 Approach to Retard Oxidation during Processing of Colloidal  $\text{Ti}_3\text{C}_2$  MXenes**  
*Touseef Habib, Smit Shah, Yexiao Chen, Wanmei Sun, Miladin Radovic, and Micah J. Green*
- P.5 Ab-initio Investigation of Dimethyl Disulfide as an Additive for Lithium-Sulfur Batteries**  
*Ethan P. Kamphaus and Perla B. Balbuena*
- P.6 Ferrocene-Based Redox Switches for Reversible Single-Molecule Magnet Behavior in Dysprosium(III) and Erbium(III) Bis-diamidoferrocene Complexes**  
*Courtney M. Dickie, Alexander L. Laughlin, Joshua D. Wofford, Nattamai S. Bhuvanesh, and Michael Nippe*

### Process Systems Engineering

- P.7 Systematic Process Intensification Using Building Blocks**  
*Salih Emre Demirel, Jianping Li, and M. M. Faruque Hasan*
- P.8 A Novel Derivative-Free Optimization Method on Single Dimension Projection**  
*Ishan Bajaj and M. M. Faruque Hasan*
- P.9 Modeling, Simulation and Optimization of Hybrid Adsorption-Reaction Systems**  
*Akhil Arora, Ishan Bajaj, Shachit S. Iyer, and M. M. Faruque Hasan*
- P.10 Toward a Systematic Framework for the Synthesis of Safely Operable Process Intensification Systems**  
*Yuhe Tian, M. Sam Mannan, and Efstratios N. Pistikopoulos*

### Pharmaceuticals and Bioengineering

- P.11 Effect of Carbon Dioxide-Sustained Adsorption using Ion-Exchange Resin on Mixed-Acid Fermentation**  
*Haoran Wu, Samarпита Roy, Kefan Yang, and Mark Holtzapple*

### Process Safety Engineering

- P.12 Fire Incidents in Offshore Oil and Gas Rigs: Analyses of Incident Investigation Reports**  
*Zohra Halim, Sunder Janardanan, Tatiana Flechas and M. Sam Mannan*
- P.13 Calorimetry Studies of Benzoyl Peroxide**  
*Yueqi Shen and M. Sam Mannan*

**P.14 Safety Assessment of Secondary Alcohol Oxidation with Hydrogen Peroxide**

*Yue Sun, Lei Ni, Maria Papadaki, Wen Zhu, Juncheng Jiang and M. Sam Mannan*

**P.15 Studying the Effects of Obstacle Configuration and Fire Suppressants on Flame Propagation Regimes**

*Cassio B. Ahumada, Eric Petersen, and M. Sam Mannan*

**Microelectronics and Nanotechnology**

**P.16 Predicting the Stability of Pt<sup>II</sup>-Based Molecular Gyroscope Isomers**

*Andreas Ehnbohm, Lisa M. Pérez, Michael B. Hall, and John A. Gladysz*

**P.17 Study on the Interfacial Interaction between Carbon Nanotubes and Catalyst, and the Effect in Tube Diameter**

*Mauricio Carvajal Diaz and Perla B. Balbuena*

## POSTER SESSION II

MSC 2300A

1:00 P.M. – 2:00 P.M.

### Advanced Materials

**P.18 Electrochemical Investigations of Electroactive Redox Polymer for Use in Energy Storage Devices**

*Kasturi Sarang, Hysoung An, Andrea Miranda, Jodie L. Lutkenhaus, and Rafael Verduzco*

**P.19 Saturated N-heterocyclic Cationic Polymers: Synthesis and Stability**

*Rui Sun and Yossef A. Elabd*

**P.20 High-Resolution Scalable Propylene/Propane Separation for ZIF-8 Polycrystalline Membranes on Ceramic Tubular Support**

*Jingze Sun and Hae-Kwon Jeong*

**P.21 Application of Electrochemical Impedance Spectroscopy for the Study of Degradation Behavior of Nanowire Thin Films in Simulated Industrial Environments**

*Pranav Kannan, M. Sam Mannan, and Sreeram Vaddiraju*

**P.22 Cone Calorimeter Analysis of Flame Retardant Poly(styrene) Nanocomposite**

*Lubna Ahmed, Bin Zhang, Ruiqing Shen, Zhengdong Cheng, Qingsheng Wang, and M. Sam Mannan*

**P.23 Combined High Stretchability and Gas Barrier in Hydrogen-Bonded Multilayer Nanobrick Wall Thin Films**

*Shuang Qin, Yixuan Song, Michael E. Floto, and Jaime C. Grunlan*

### Process Systems Engineering

**P.24 Advancing the Production of Olefins and Aromatics from Natural Gas via Methanol: Chemical Looping for Syngas Generation**

*William W. Tso, C. Doga Demirhan, Alexander M. Niziolek, Onur Onel, Christodoulos A. Floudas, and Efstratios N. Pistikopoulos*

**P.25 Fault Detection and Diagnosis of Continuous Processes via Non-linear Support Vector Machine based Feature Selection**

*Melis Onel, Chris A. Kieslich, Yannis A. Guzman, Christodoulos A. Floudas, and Efstratios N. Pistikopoulos*

**P.26 Multi-scale Optimization of a Novel Separation and Storage Technology for Natural Gas**

*Shachit S. Iyer, Salih E. Demirel, and M. M. Faruque Hasan*

**P.27 Multi-objective Stochastic Optimization for Preventive Maintenance Planning in Chemical Plants**

*Christopher Gordon, Monir Ahammad, and M. Sam Mannan*

### Safety Engineering

**P.28 Identify Weak Signals Using Data Mining Techniques**

*Mengxi Yu, Noor Quddus, and M. Sam Mannan*

**P.29 Mapping Review of Reactive Chemicals Hazards Research**

*Hallie Graham and M. Sam Mannan*

**P.30 Developing Probabilistic Barrier Failure Models to Predict Kicks while Drilling**

*Nafiz Tamim, Delphine Laboureur, A. Rashid Hasan and M. Sam Mannan*

**P.31 Thermal Decomposition of Mono-Nitrated Toluene (MNT) with Additives**

*Wen Zhu and Chad V. Mashuga*

**P.32 Optimization of Flame Retardants on Commercial Aircrafts**

*Mazdak Mina and M. Sam Mannan*

**Energy Systems**

**P.33 Formation of Multi-layer Graphene Nanosheets with Strong Sulfur-Carbon Interaction and Enhanced Sulfur Reduction Zones for Lithium-Sulfur Battery Cathodes**

*Saul Perez Beltran and Perla B. Balbuena*

**Environmental Engineering**

**P.34 Magnetically Driven Functionalized Nanoplatelets Pickering Emulsion for Removal of Oil Contaminants from Water**

*Dali Huang, Minxiang Zeng, Lecheng Zhang, Arun Sabapathy, Janet Sajan, and Zhengdong Cheng*

**Pharmaceuticals and Bioengineering**

**P.35 Microfluidic Microbiologically Influenced Corrosion (M-MIC) Models**

*Susmitha Purnima Kotu, M. Sam Mannan and Arul Jayaraman*





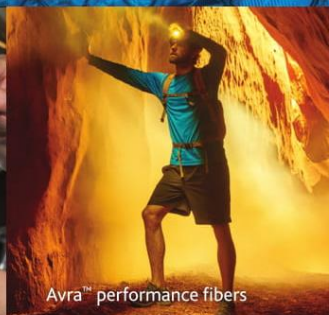
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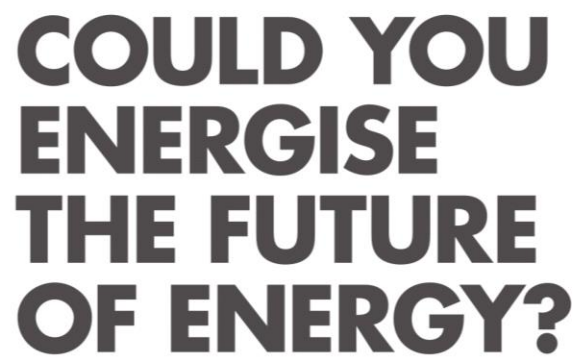
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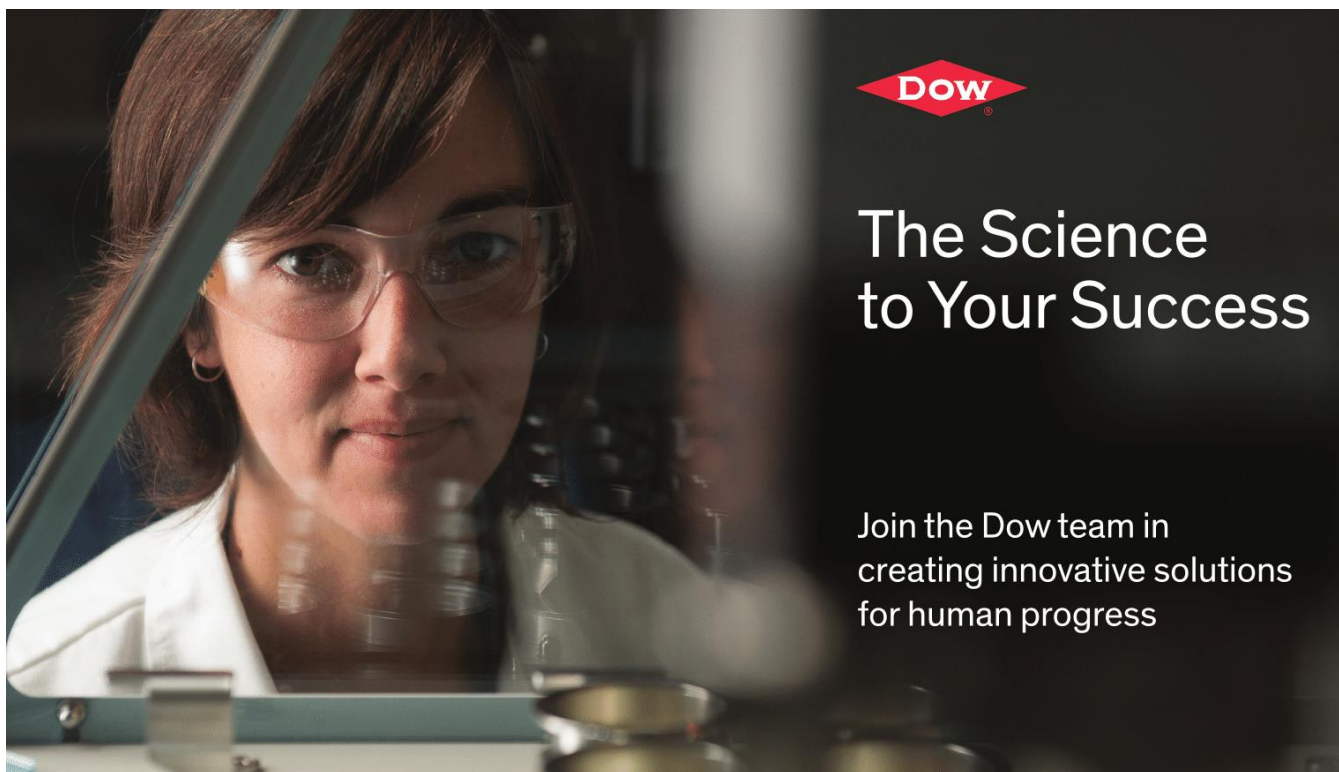
## Chemical Engineering Graduate Student Association



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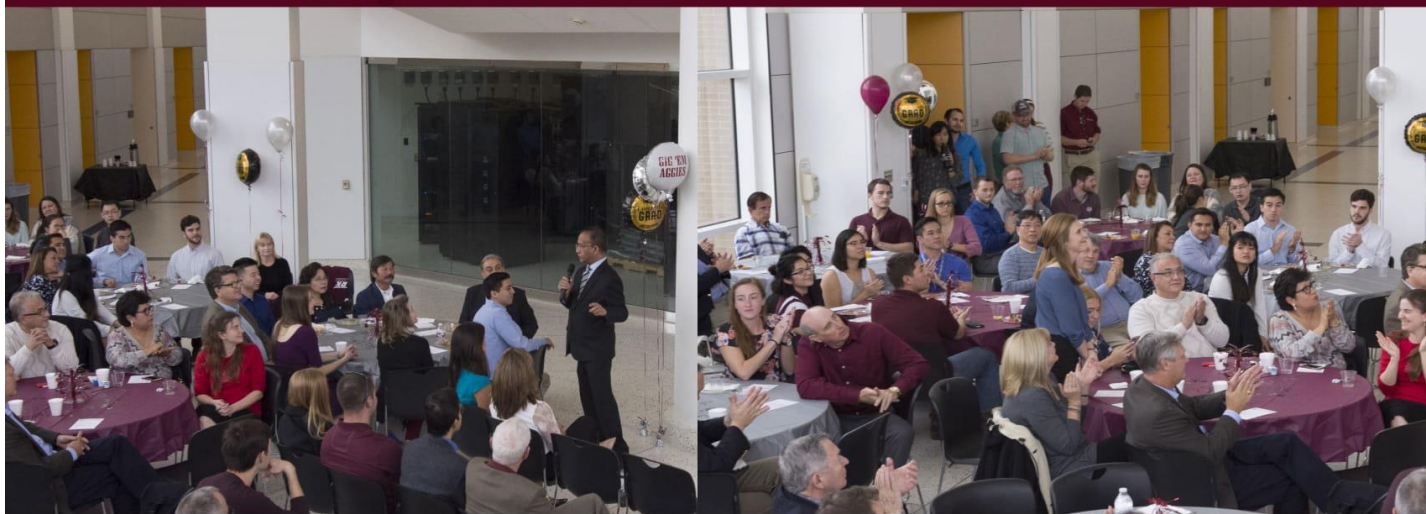
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The Artie McFerrin Department of Chemical Engineering is one of the top rated chemical engineering departments in the world. It is also one of the largest, fully accredited chemical engineering programs in the country. The department has become a prolific chemical engineering research hub, with the faculty producing more than 200 refereed journal publications in 2017.

Located in the 205,000 square-foot, Jack E. Brown Chemical Engineering Building, the department provides its students and faculty members access to the latest resources, including 88 research and teaching facilities, six general classrooms, 13 conference rooms, and four computer laboratories.

## Research

The Artie McFerrin Department of Chemical Engineering at Texas A&M University has faculty engaged in a wide breadth of studies ranging from highly applied research in the areas of biomass utilization, process safety and hydrocarbon processing to very fundamental research in nanotechnology, life sciences, process systems engineering and molecular simulation. The ultimate goal of the research is to positively impact society by providing new knowledge.

## Department Research Areas

- Biomedicine | Biomolecules
- Biofuels | Biotechnology
- Catalysis
- Complex Fluids | Microfluidics | Soft Matter
- Computational Chemical Engineering
- Energy
- Environmental | Sustainability
- Materials | Microelectronics
- Multiscale Systems Engineering
- Nanotechnology
- Process Safety | Process Systems Engineering
- Reaction Engineering
- Thermodynamics

## Department Head

**M.Nazmul Karim** | Professor | T. Michael O'Connor Chair II  
nazkarim@tamu.edu

## Enrollment

<b>Total Enrollment</b>	<b>1,029</b>
Undergraduate	793
Graduate	236
Master's	96
Ph.D.	140

## Faculty

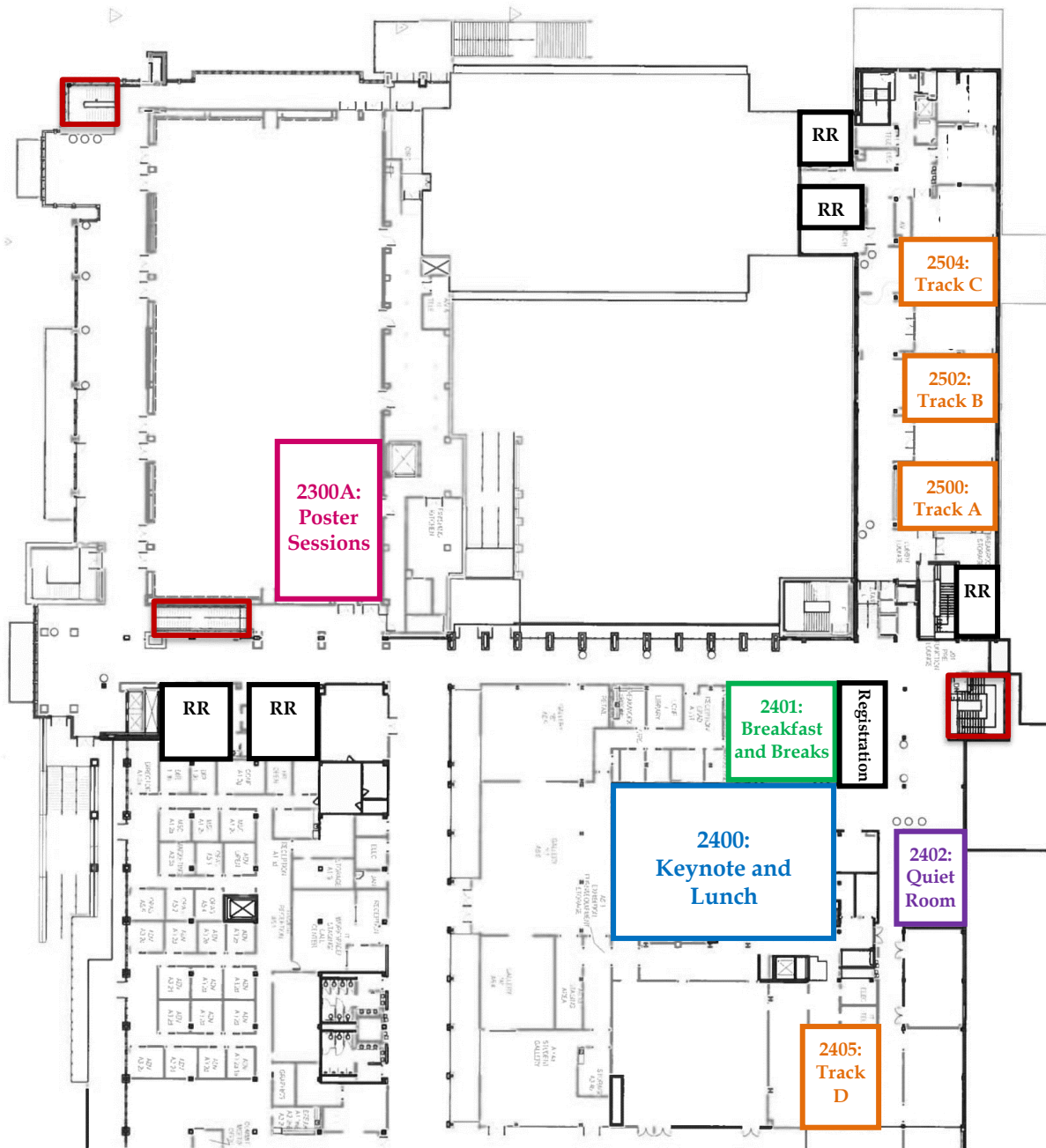
<b>Total Faculty</b>	<b>36</b>
Professors	13
Endowed Chairs	5
Endowed Professorships	7
Associate Professors	7
Assistant Professors	6
Research Assistant Professors	1
Lecturers/Senior Lecturers	4
Professors of Practice	2
Senior Professors	3
Referred Journal Publications	251

## Student Gender Diversity

Female	39%
Male	61%



# BUILDING LAYOUT



Memorial Student Center (MSC) 2<sup>nd</sup> Floor

**2400: Keynote Address and Lunch Reception**

**2401: Breakfast and Breaks**

**2300A: Poster Sessions**

**2500: Track A**

**2502: Track B**

**2504: Track C**

**2405: Track D**

**2402: Quiet Room**

**Emergency Exits Marked**

4<sup>th</sup> Chemical Engineering Graduate Student Association  
**ANNUAL RESEARCH SYMPOSIUM**

Friday, March 10, 2017 | 8:00 am - 5:30 pm | MSC, Texas A&M University



## TABLE OF CONTENTS

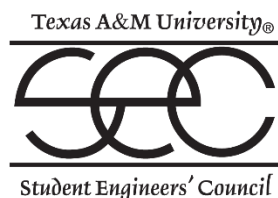
SPONSORS.....	2
WELCOME .....	3
ADVISORY COMMITTEE.....	3
ORGANIZING COMMITTEE.....	3
SCHEDULE.....	4
KEYNOTE ADDRESS - Dr. Angela Summers .....	5
INDUSTRIAL SPEAKER – Dr. Cesar Granda .....	6
INDUSTRIAL SPEAKER – Dr. Carl Willis.....	7
INDUSTRIAL SPEAKER – Dr. Leo H. Chiang.....	8
Track A – MSC 2500.....	10
Track B – MSC 2502 .....	10
Track C – MSC 2504.....	11
Track D – MSC 2405.....	11
Poster Session I.....	12
Poster Session II.....	14

## SPONSORS

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**Dr. Jim Harris**



## **WELCOME**

On behalf of the organizing committee we extend you a warm welcome to College Station and the 4<sup>th</sup> Annual Research Symposium. The purpose of the symposium is to showcase the research conducted in the department and provide students with an opportunity to present their research to industrial representatives. We gratefully acknowledge the sponsorship provided by Ascend Performance materials, Shell, Dow, Texas A&M Division of Research, The Kaneka Foundation, Dr. Jim Harris, BASF and Texas A&M Student Engineering Council. This symposium represents the ideal environment for the exchange of ideas to aid in the advancement of science and technology. We wish all the participants a productive and enjoyable event.

## **ADVISORY COMMITTEE**

**DR. ARUL  
JAYARAMAN**

**DR. M. SAM  
MANNAN**

**DR. HOMA  
KHOSRAVIAN**

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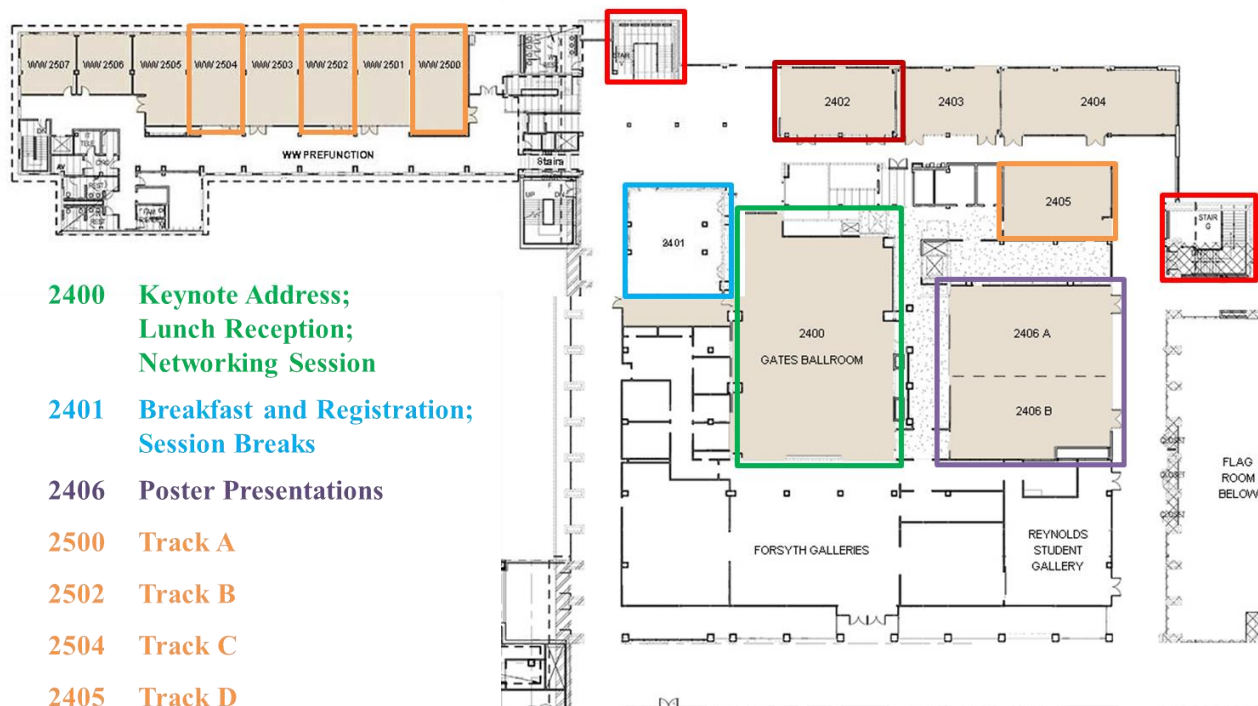
# SCHEDULE

Time	Event			
8:00 – 9:00	Breakfast and Registration			
9:00 – 9:15	Opening Remarks by Pritishma Lakhe and Dr. Nazmul Karim			
9:15 – 9:45	Keynote Address by Dr. Angela Summers			
9:45 – 10:00	Break			
	Track A- MSC 2500	Track B- MSC 2502	Track C- MSC 2504	Track D- MSC 2405
10:00 – 10:20	● Nirup Nagabandi	● Pilar Suarez-Martinez	● Melis Onel	● Shachit Iyer
10:20 – 10:40	● Yixuan Song	● Susmitha Kotu	● Ishan Bajaj	● Utkarsh Shah
10:40 – 11:00	● Tianyu Yuan	● Hyosung An	● Chiranjivi Botre	● Priya Balasubramanian
11:00 – 12:15	Poster Session I			
12:15 – 1:30	Lunch			
1:30 – 2:45	Poster Session II			
2:45 – 3:15	Dr. Carl Willis	Dr. Cesar Granda	Dr. Leo Chiang	
3:15 – 3:30	Break			
3:30 – 3:50	● Lubna Ahmed	● Ravi Chawla	● Perna Jain	● Kevin Topolski
3:50 – 4:10	● Bharatvaaj Ravi	● Lecheng Zhang	● Syeda Zohra Halim	● Gerald Oguremem
4:10 – 5:10	Networking Session			
5:10 – 5:20	Closing Remarks and Awards by Monica Hwang			

## Research Focus

● Advanced Materials
 ● Safety Engineering
 ● Bioengineering
 ● Process Systems Engineering

## BUILDING LAYOUT



**2400** Keynote Address;  
Lunch Reception;  
Networking Session

**2401** Breakfast and Registration;  
Session Breaks

**2406** Poster Presentations

**2500** Track A

**2502** Track B

**2504** Track C

**2405** Track D

**2402** Quiet Room

Emergency exits are marked



## KEYNOTE ADDRESS - Dr. Angela Summers



**Dr. Angela Summers, Ph.D.**  
**President, SIS-TECH Solution, LP**

### **From Sci-fi Nerd to Engineer to Vintner – a chemical engineer's journey**

Dr. Angela Summers started SIS-TECH over 15 years ago with \$1,000 and a desire to stop process safety incidents. With over 100 employees and contractors, SIS-TECH has become a respected and trusted provider of services and systems for process safety and critical control applications of automation systems. She has over 30 years of experience in instrumentation and controls, process design, and environmental pollution controls. Dr. Summers holds a PhD in chemical engineering. She was named an Engineering Fellow of the University of Alabama and a Centennial Fellow of its chemical engineering department (top 100 graduates in 1st 100 years of the program).

## INDUSTRIAL SPEAKER – Dr. Cesar Granda



**Dr. Cesar Granda, Ph.D.**  
**CTO, Earth Energy Renewables**

### **Being Pragmatic About Caring for the Environment through Chemical Engineering**

Certain scientific topics can be the subject of endless political controversy despite the fact that scientists and engineers should be above politics. Caring for the environment happens to be one of such topics, where the government can take very different approaches depending on who is in charge. As chemical engineers, we have the opportunity to deliver pragmatism to the debate by offering profitable solutions to the problem, rather than approaches that many times can be a burden on the economy and are not sustainable in the long run.

Earth Energy Renewables is developing a technology, which can sustainably attain a profitable outcome while solving environmental problems and caring for the environment. This technology, which has its roots at the Texas A&M University Chemical Engineering Department, employs Biotechnology and conventional Chemical Engineering. The process uses a mixed consortium of naturally occurring microorganisms to ferment or digest any biodegradable material, such as organic wastes (e.g., organic garbage, wastewater, organic effluents, and agricultural residues) or crops (e.g., corn, sorghum, grass) and produce valuable chemical products. These chemical products, which are organic acids (e.g., acetic, propionic, butyric acids) are recovered from the fermentation effluent and purified. As such, these acids can be commercialized into a well-established market allowing the company to become profitable and self-sufficient. These acids are also well-established intermediates to produce other valuable chemical products, such as ketones, esters, primary and secondary alcohols, and even biofuels, such as gasoline and jet fuel, which represent a good opportunity for substantial growth and sustainability as well as for a significant positive impact on the environment.

## INDUSTRIAL SPEAKER – Dr. Carl Willis



**Dr. Carl Willis, Ph.D.**  
**Research Fellow, Kraton Polymers**

### **Ion Containing Block Copolymers**

In 2010, Kraton Polymers started producing a grade line of ion containing, styrenic block copolymers under the tradename of Nexar® Polymers. The polymers are made by a 3 step process. In the first step, a 5 block copolymer is prepared by a living anionic polymerization technology; the living anionic polymerization method affords block copolymer segments that are nearly monodispersed in molecular weight. In the second step, the polymer is selectively hydrogenated to remove C=C unsaturation. In the final step, the pentablock copolymer is selectively sulfonated in the polystyrene block (center segment).

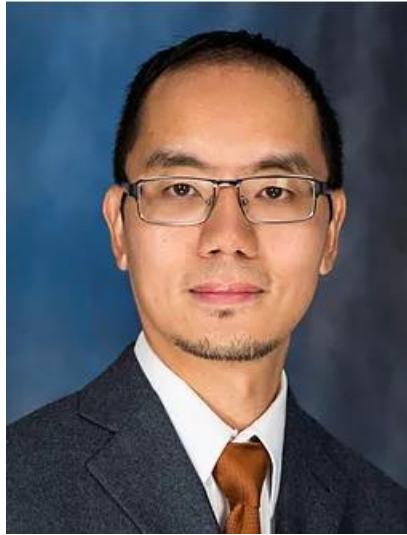
The sulfonated polystyrene segment in these polymers gives the material unique structure and unusual performance features. Solutions of these polymers tend to be structured which gives rise to the interesting rheological properties observed for the solutions.

The Nexar Polymer solutions have been cast into membranes which have found utility in energy recovery ventilation applications.

Additionally, the Nexar Polymer solutions have also been printed onto fabrics and the resulting coated fabrics made into garments that provide an improved micro-climate for the wearer. This technology provides a mechanism for cooling the person wearing the garment when working in a hot climate.

This presentation will focus on the science that supports these technologies.

## INDUSTRIAL SPEAKER – Dr. Leo H. Chiang



**Dr. Leo H. Chiang, Ph.D.**

**Associate Technology Director, The Dow Chemical Company**

### **Advances in Big Data Analytics at The Dow Chemical Company**

In the Big Data era, Dow is collecting large volume of data (in the order of terabytes each day) of various kinds such as process data, experimental lab data, business transaction data, image data, and text data. While these data present a unique opportunity to improve process understanding and bring value to Dow, it is often challenging to use the right data and right tools to make the right decisions in real-time. This talk highlights recent advancements in the big data analytics journey at Dow in the areas of Enterprise Manufacturing Intelligence, multivariate analysis, on-line fault detection, inferential sensors, and batch data analytics.



**NOTES**

# Oral Presentations

## Track A – MSC 2500

Track	Morning	Presentation
A1	10:00 – 10:20	SILVER METAL-ORGANIC-INORGANIC COMPOSITES AS THERMAL INTERFACE MATERIALS <i>Nirup Nagabandi, Cengiz Yegin, Jun Kyun Oh and Mustafa Akbulut</i>
A2	10:20 – 10:40	HIGH OXYGEN GAS BARRIER IN MULTILAYER THIN FILMS THROUGH PH MANIPULATION OF MONTMORILLONITE CLAY NANOPATELETS <i>Yixuan Song, David A. Hagen and Jaime C. Grunlan</i>
A3	10:40 – 11:00	VERSATILE THERMOCHROMIC SUPRAMOLECULAR MATERIALS BASED ON CHARGE TRANSFER INTERACTIONS <i>Tianyu Yuan, Mariela Vazquez, Mark A. Olson and Lei Fang</i>

Track	Afternoon	Presentation
Industry	2:45 – 3:15	ION CONTAINING BLOCK COPOLYMERS <i>Dr. Carl Willis, Research Fellow, Kraton Polymers</i>
A4	3:30 – 3:50	FLAMMABILITY STUDIES BY CONE CALORIMETER ANALYSIS OF SILICA CROSS-LINKED POLY (METHYL METHACRYLATE) <i>Lubna Ahmed, Ruiqing Shen, Logan Hatanaka, Bin Zhang, Sam Mannan, Zhengdong Cheng and Qingsheng Wang</i>
A5	3:50 – 4:10	STUDY OF FACTORS THAT AFFECT DUST EXPLOSION CHARACTERISTICS OF FIBROUS DUST MATERIALS <i>Bharatvaaj Ravi, M. Sam Mannan and Chad Mashuga</i>

## Track B – MSC 2502

Track	Morning	Presentation
B1	10:00 – 10:20	SPRAY-ON POLYMER-CLAY MULTILAYERS AS A SUPERIOR ANTICORROSION METAL PRETREATMENT <i>Pilar C. Suarez-Martinez, Jerome Robinson, Hyosung An, Robert C. Nahas, Douglas Cinoman and Jodie L. Lutkenhaus</i>
B2	10:20 – 10:40	MODIFIED MICROFLUIDIC FLOW SYSTEM FOR ASSESSMENT OF MICROBIOLOGICALLY INFLUENCED CORROSION <i>Susmitha Purnima Kotu, Sam Mannan and Arul Jayaraman</i>
B3	10:40 – 11:00	CONDUCTING BLOCK COPOLYMER BATTERY ELECTRODE BINDERS COMPARED AGAINST THEIR HOMOPOLYMER BLEND ANALOGS <i>Hyosung An, Xiaoyi Li, Cody Chalker, Maria Stracke, Rafael Verduzco and Jodie L. Lutkenhaus</i>

Track	Afternoon	Presentation
Industry	2:45 – 3:15	BEING PRAGMATIC ABOUT CARING FOR THE ENVIRONMENT THROUGH CHEMICAL ENGINEERING <i>Dr. Cesar Granda, CTO, Earth Energy Renewables</i>
B4	3:30 – 3:50	TORQUE-DEPENDENT MOTOR REMODELING AND MECHANOSENSING IN E. COLI <i>Ravi Chawla, Katie M. Ford and Pushkar P. Lele</i>
B5	3:50 – 4:10	NOVEL JANUS NANOPATELETS FOR ENHANCED OIL RECOVERY <i>Lecheng Zhang, Mingxiang Zeng and Zhengdong Cheng</i>

## Track C – MSC 2504

Track	Morning	Presentation
C1	10:00 – 10:20	BIG DATA APPROACH TO FAULT DETECTION AND DIAGNOSIS IN BATCH PROCESSES USING NONLINEAR SVM-BASED FEATURE SELECTION <i>Melis Onel, Chris A. Kieslich, Yannis A. Guzman Christodoulos A. Floudas and Efstratios N. Pistikopoulos</i>
C2	10:20 – 10:40	NOVEL METHOD FOR DERIVATIVE-FREE OPTIMIZATION BASED ON PARAMETRIC APPROACH <i>Ishan Bajaj and M. M. Faruque Hasan</i>
C3	10:40 – 11:00	PROCESS MONITORING OF NONLINEAR INDUSTRIAL PROCESSES USING MULTISCALE REPRESENTATION OF IMPROVED KERNEL PARTIAL LEAST SQUARE (KPLS) TECHNIQUE <i>Chiranjivi Botre, Majdi Mansouri, Mohamed N. Nounou, Hazem N. Nounou and M. Nazmul Karim</i>

Track	Afternoon	Presentation
Industry	2:45 – 3:15	ADVANCES IN BIG DATA ANALYTICS AT THE DOW CHEMICAL COMPANY <i>Dr. Leo H. Chiang, Associate Technology Director, Dow</i>
C4	3:30 – 3:50	RESILIENCE-BASED LOSS OF CONTAINMENT (LOC) EVENTS PREDICTION ANALYSIS FOR POLY VINYL CHLORIDE PROCESS SYSTEM: UNCERTAINTY QUANTIFICATION <i>Prerna Jain and M. Sam Mannan</i>
C5	3:50 – 4:10	CUMULATIVE RISK ASSESSMENT MODEL TO DETERMINE INCREASED RISK DUE TO IMPAIRED BARRIERS <i>S. Zohra Halim and M. Sam Mannan</i>

## Track D – MSC 2405

Track	Morning	Presentation
D1	10:00 – 10:20	DESIGN AND OPTIMIZATION OF MODULAR TECHNOLOGY FOR INTEGRATED CARBON CAPTURE & CONVERSION OF CO <sub>2</sub> USING METHANE SOURCES <i>Shachit S. Iyer, Ishan Bajaj, Priyadarshini Balasubramanian and M. M. Faruque Hasan</i>
D2	10:20 – 10:40	AN IMPROVED APPROACH FOR ROBUST SCHEDULING UNDER UNCERTAINTY <i>Utkarsh D. Shah, Yannis A. Guzman, Logan R. Matthews and Christodoulos A. Floudas</i>
D3	10:40 – 11:00	CO <sub>2</sub> CAPTURE AND CONVERSION TO CHEMICALS VIA SYNGAS: SUPERSTRUCTURE-BASED PROCESS SYNTHESIS, MODELING, AND OPTIMIZATION <i>Priyadarshini Balasubramanian, Ishan Bajaj and M. M. Faruque Hasan</i>

Track	Afternoon	Presentation
D4	3:30 – 3:50	ANCHOR-TENANT MODELS FOR THE SYNTHESIS OF ECO-INDUSTRIAL PARKS THROUGH CARBON-HYDROGEN-OXYGEN SYMBIOSIS NETWORKS <i>Kevin Topolski, Mohamed Noureldin, and Mahmoud El-Halwagi</i>
D5	3:50 – 4:10	DYNAMIC MODELING AND OPTIMIZATION OF RENEWABLE HIGH-PRESSURE PEM HYDROGEN PRODUCTION AND STORAGE <i>Gerald S. Ogumerem and Efstratios N. Pistikopoulos</i>

# Poster Session I

MSC 2406

11:00 A.M. – 12:15 P.M.

## Advanced Materials

- P.1**    **Aramid Nanofiber/Graphene/Carbon Nanotube Composite Electrodes for Structural Energy and Power**  
*Anish Patel, John Harris and Jodie L. Lutkenhaus*
- P.2**    **Solid-state Synthesis and Thermoelectric Properties of Magnesium Silicide**  
*Azhar Ali, Venkata Vasiraju, Yixi Chen and Sreeram Vaddiraju*
- P.3**    **Electric Field Induced Birefringence in Isotropic Suspensions of Nanoplates**  
*Carlos Mejia, Abhijeet Shinde, Ivan Dozov, Padetha Tin, Patrick Davidson and Zhengdong Cheng*
- P.4**    **Biodegradable 3D Printed Oil Absorbents with Tunable Capillary Architectures**  
*Duanduan Han and Victor Ugaz*
- P.5**    **Electrolyte Structure and Behavior of Polysulfide species in Lithium-Sulfur Batteries**  
*Ethan P. Kamphaus and Perla B. Balbuena*
- P.6**    **Rapid Microwave-assisted Synthesis of Hybrid Zeolitic-Imidazolate Frameworks with Mixed Metals and Mixed Linkers**  
*Febrian Hillman, John Zimmerman, Seung-Min Paek, Mohamad R. A. Hamid, Woo T. Lim and Hae-Kwon Jeong*
- P.7**    **Liquid Surfactants for Processing Boron Nitride Nanosheets (BNNSs)**  
*Touseef Habib, Dinesh Sundaravadivelu Devarajan, Fardin Khabaz, Dorsa Parviz, Thomas C. Achee, Rajesh Khare and Micah J. Green*

## Process Systems Engineering

- P.8**    **Model order reduction of parabolic PDE systems based on temporally-local Dynamic mode decomposition with control**  
*Abhinav Narasingam and Joseph Sang-Il Kwon*
- P.9**    **Global Optimization of Constrained Grey-Box Models for Well Injection and Production**  
*Burcu Beykal, Fani Boukouvala, Nadav Sorek, Hardikkumar Zalavadia, Eduardo Gildin, Christodoulos A. Floudas and Efstratios N. Pistikopoulos*
- P.10**    **Improved Data-Driven Mathematical Modeling and Global Optimization Framework: An Application in Refinery Planning Operations**  
*C. Doga Demirhan, Fani Boukouvala Kyungwon, Kim Hyeju Song, Efstratios N. Pistikopoulos and Christodoulos A. Floudas*
- P.11**    **Simultaneous Process Network Synthesis and Process Intensification Using Grid Superstructure**  
*Jianping Li, Salih Emre Demirel and M. M. Faruque Hasan*

## Pharmaceuticals and Bioengineering

- P.12**    **Binding of Cholera toxin subunit B with heterogeneous glycolipids on cell mimicking surfaces**  
*Pratik Krishnan, Akshi Singla, Chin-An Lee, Joshua D. Weatherston, Nolan C. Worstell and Hung-Jen Wu*



**P.13 The production of high-value intracellular compounds using a process synthesis framework**

*Alexander M. Sabol, Maria-Ona Bertran, Jonathan P. Raftery, Rafiqul Gani and M. Nazmul Karim*

**P.14 Modeling LPS-induced TNF- $\alpha$  Production in Macrophages**

*Dongheon Lee, Yufang Ding, Arul Jayaraman and Joseph Sangil Kwon*

### **Safety Engineering**

**P.15 Incorporating Human Factors Engineering Methods in the System Life Cycle of Offshore Oil and Gas Industries**

*Changwon Son, Syeda Zohra Halim, Yogesh Koirala and M. Sam Mannan*

**P.16 Dust-Gas Hybrid Minimum Ignition Energy Prediction**

*Haitian Han and Chad V. Mashuga*

**P.17 Aerosol generation approach and combustion simulation**

*Shuai Yuan and M. Sam Mannan*

### **Energy**

**P.18 Countercurrent Enzymatic Saccharification and Continuum Particle Distribution Model of Pretreated Corn Stover**

*Chao Liang, Mark Holtzaple and M. Nazmul Karim*

### **Environmental Engineering**

**P.19 High-flux hybrid membranes for effective oil-water separation from oil-contaminated water**

*Glenn Zeng, Lecheng Zhang, Dali Huang and Zhengdong Cheng*

### **Microelectronics and Nanotechnology**

**P.20 Using black particles as an additive to produce tunable structural colors with high color contrast in photonic crystals**

*Dali Huang, Minxiang Zeng, Lecheng Zhang and Zhengdong Cheng*

**P.21 Enhancing photocatalytic CO<sub>2</sub> reduction by coating an ultrathin Al<sub>2</sub>O<sub>3</sub> layer on oxygen deficient TiO<sub>2</sub> nanorods through atomic layer deposition**

*Huilei Zhao and Ying Li*

# Poster Session II

MSC 2406

1:30 P.M. – 2:45 P.M.

## Advanced Materials

**P.22 Synthesis and Characterization of CdIF-1: A Cadmium Version of ZIF-8**

*Jingze Sun, Liya Semenchenko, and Hae-Kwon Jeong*

**P.23 Computational Study of the Adsorption of a Phenanthrene Derivative over a Model Zeolite**

*Monica M. Garnica-Mantilla, Ana E. Torres-Hernández, Luis E. Camacho-Forero, Carlos M. Celis-Cornejo, Gustavo E. Ramírez-Caballero and Perla B. Balbuena*

**P.24 PIL-Derived Carbon**

*Rui Sun, Kelly M. Meek and Yossef A. Elabd*

**P.25 Water-Based Assembly of Polymer-Metal Organic Framework (MOF) Functional Coatings**

*Souvik De, Manjula I. Nandasiri, Herbert T. Schaef, Benard Peter McGrail, Satish K. Nune and Jodie L. Lutkenhaus*

**P.26 Porous nanomaterials with high performance energy storage**

*Wanmei Sun and Micah Green*

**P.27 The Effect of Water on the Thermal Transition Observed in Poly(allylamine hydrochloride)-Poly(acrylic acid) Complexes**

*Yanpu Zhang, Ran Zhang, Maria Sammalkorpi and Jodie L. Lutkenhaus*

## Process Systems Engineering

**P.28 Simultaneous Design and Control of a Binary Distillation Column**

*Baris Burnak, Justin Katz, Nikolaos A. Diangelakis and Efstratios N. Pistikopoulos*

**P.29 Modeling of hydraulic fracturing and design of online optimal pumping schedule to achieve uniform proppant concentration**

*Prashanth Siddhamshetty and Joseph Sangil Kwon*

**P.30 Systematic Process Intensification Using Building Blocks**

*Salih Emre Demirel, Jianping Li and M. M. Faruque Hasan*

**P.31 Systematic Analysis and Optimization of Energy-Water Nexus**

*Spyridon D. Tsolas, M. Nazmul Karim and M. M. Faruque Hasan*

**P.32 Natural Gas to Liquid Transportation Fuels Utilizing Chemical Looping Technologies for Syngas Generation: Process Synthesis and Global Optimization**

*William W. Tso, Alexander M. Niziolek, Onur Onel and Christodoulos A. Floudas*

**P.33 Monetization of Stranded Gas through Ammonia and Urea Production**

*Zehao Gou, Debalina Sengupta, Mike Dou and M.M. El-Halwagi*

## Safety Engineering

**P.34 The Integration of Design, Control, and Safety**

*Denis Su-Feher, Yogesh Koirala, Efstratios Pistikopoulos and M. Sam Mannan*

**P.35 A systematic approach to alarm design with application to Tennessee Eastman Problem**

*Joshiba Ariamuthu Venkidasalapathy, Costas Kravaris and M. Sam Mannan*

**P.36 A Leading Indicators-based Decision Support Tool to Predict Blowout Events**

*Nafiz Tamim, Delphine Laboureur, M. Sam Mannan and A. Rashid Hasan*

**P.37 A New Semi-Automated HAZID Method for More Comprehensive Identification of Hazardous Scenarios**

*Sunhwa Park, Yan-Ru Lin and M. Sam Mannan*

**Energy**

**P.38 In-situ Mechanistic Investigation of an Organic Radical Polymer Cathode on Interfacial Charge and Mass Transfer**

*Shaoyang Wang, Fei Li and Jodie Lutkenhaus*

**Environmental Engineering**

**P.39 Advanced heavy gas dispersion model with less time and higher near-field accuracy than CFD-based simulation**

*Jiayong Zhu, Delphine Laboureur, and M. Sam Mannan*

**Microelectronics and Nanotechnology**

**P.40 Template-free 3D titanium carbide (MXene) particles crumpled by capillary forces**

*Smit. A. Shah, T. Habib, H. Gao, P. Gao, W. Sun, M. J. Green and M. Radovic*

**P.41 Large-Scale Synthesis of Byproduct-Free Semiconducting Nanomaterials: Direct Conversion of Highly Porous Zn Pellets to Zn<sub>3</sub>P<sub>2</sub> Nanowires**

*Yixi Chen, Rakesh Polinnaya, Pranav Kannan, Azhar Ali and Sreeram Vaddiraju*



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The Artie McFerrin Department of Chemical Engineering at Texas A&M University is one of the top rated chemical engineering departments in the world. It is also one of the largest, fully accredited chemical engineering programs in the country. The department has become a prolific chemical engineering research hub, with the faculty producing more than 200 refereed journal publications in 2016.

Located in the 205,000 square-foot, Jack E. Brown Chemical Engineering Building, the department provides its students and faculty members access to the latest resources, including 88 research and teaching facilities, six general classrooms, 13 conference rooms, and four computer laboratories.

## Research

The Artie McFerrin Department of Chemical Engineering at Texas A&M University has faculty engaged in a wide breadth of studies ranging from highly applied research in the areas of biomass utilization, process safety and hydrocarbon processing to very fundamental research in nanotechnology, life sciences, process systems engineering and molecular simulation. The ultimate goal of the work is to positively impact society by providing new knowledge.

## Department Research Areas

- Biomedicine | Biomolecules
- Biofuels | Biotechnology
- Catalysis
- Complex Fluids | Microfluidics | Soft Matter
- Computational Chemical Engineering
- Energy
- Environmental | Sustainability
- Materials | Microelectronics
- Multiscale Systems Engineering
- Nanotechnology
- Process Safety | Process Systems Engineering
- Reaction Engineering
- Thermodynamics

## Department Head

**M.Nazmul Karim** | Professor | T. Michael O'Connor Chair II  
nazkarim@tamu.edu

## Enrollment

<b>Total Enrollment</b>	<b>969</b>
Undergraduate	714
Graduate	255
Master's	117
Ph.D.	138

## Faculty

<b>Total Faculty</b>	<b>36</b>
Professors	15
Endowed Professors	8
Chair Holders	4
Associate Professors	8
Assistant Professors	6
Research Assistant Professors	1
Lecturers/Senior Lecturers	5
Professors Of Practice	2
Emeritus Faculty	5
Referred Journal Publications	203

## Gender Diversity

Female	37%
Male	63%