

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



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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

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Jayaraman**

**Dr. Perla  
Balbuena**

**Dr. Jodie  
Lutkenhaus**

**Dr. Katy  
Kao**

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# 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><br><i>Advanced Materials</i> | <b>Track B- MSC 2502</b><br><i>Bioengineering and Polymers</i> | <b>Track C- MSC 2504</b><br><i>Process Systems Engineering</i> | <b>Track D- MSC 2405</b><br><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<br>MSC 2500<br><i>Advanced Materials</i>  | Track B<br>MSC 2502<br><i>Bioengineering and<br/>Polymers</i>   | Track C<br>MSC 2504<br><i>Process Systems<br/>Engineering</i>   | Track D<br>MSC 2405<br><i>Computational<br/>Modeling and<br/>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><br><br><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><br><br><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><br><br><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><br><br><u>Behnaz Rahmani Didar</u> and Perla B. Balbuena            |
| 10:00 – 10:20 | <b>Micro-encapsulation with Nanoplatelet Surfactant</b><br><br><u>L. Eric Zhang</u> and Zhengdong Cheng   | <b>Modulation of Ultrasensitive Signaling in Bacteria by Viscous Load on Flagellar Motor</b><br><br><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><br><br><u>Baris Burnak</u> , Justin Katz, Nikolaos A. Diangelakis, and Efstratios N. Pistikopoulos | <b>Calorimetric Study of Graphene Oxide Thermal Stability</b><br><br><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><br><br><u>Tianyu Kelvin Yuan</u> , Lei Fang, and Mark A. Olson                                      | <b>Stochastic Modeling of CTB-GM1 Binding Kinetics</b><br><br><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><br><br><u>Jianping Li</u> , Salih Emre Demirel, and M. M. Faruque Hasan  | <b>Toward Optimal Synthesis of Renewable Ammonia and Methanol Processes</b><br><br><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<br>MSC 2500<br><br><i>Advanced Materials</i>  | Track B<br>MSC 2502<br><br><i>Bioengineering and<br/>Polymers</i>   | Track C<br>MSC 2504<br><br><i>Process Systems<br/>Engineering</i>  | Track D<br>MSC 2405<br><br><i>Computational<br/>Modeling and<br/>Process Safety</i>   |
|-------------|---|---|--|---|
| 2:10 – 2:30 | <b>Surface-Agnoistic Highly Stretchable and Bendable Conductive MXene Multilayers</b><br><br><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><br><br><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><br><br><i>Eric Bohac, Mahmoud El-Halwagi, and Debalina Sengupta</i>          | <b>Improved Flare Radiation Criteria in Terms of Solar Radiation Contribution</b><br><br><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><br><br><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><br><br><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><br><br><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><br><br><i>Srikanth Panyaram and Benjamin Wilhite</i>                             |
| 2:50 – 3:10 | <b>High Efficient Oil-Water Separation using Surface-Programmable Membranes</b><br><br><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><br><br><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><br><br><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><br><br><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*



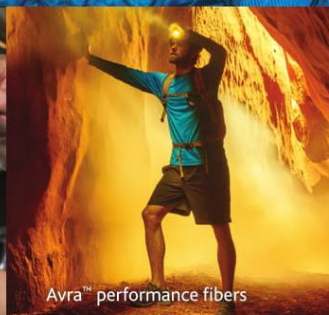
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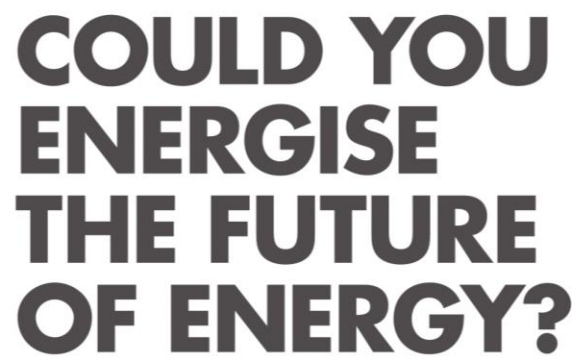
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## Chemical Engineering Graduate Student Association


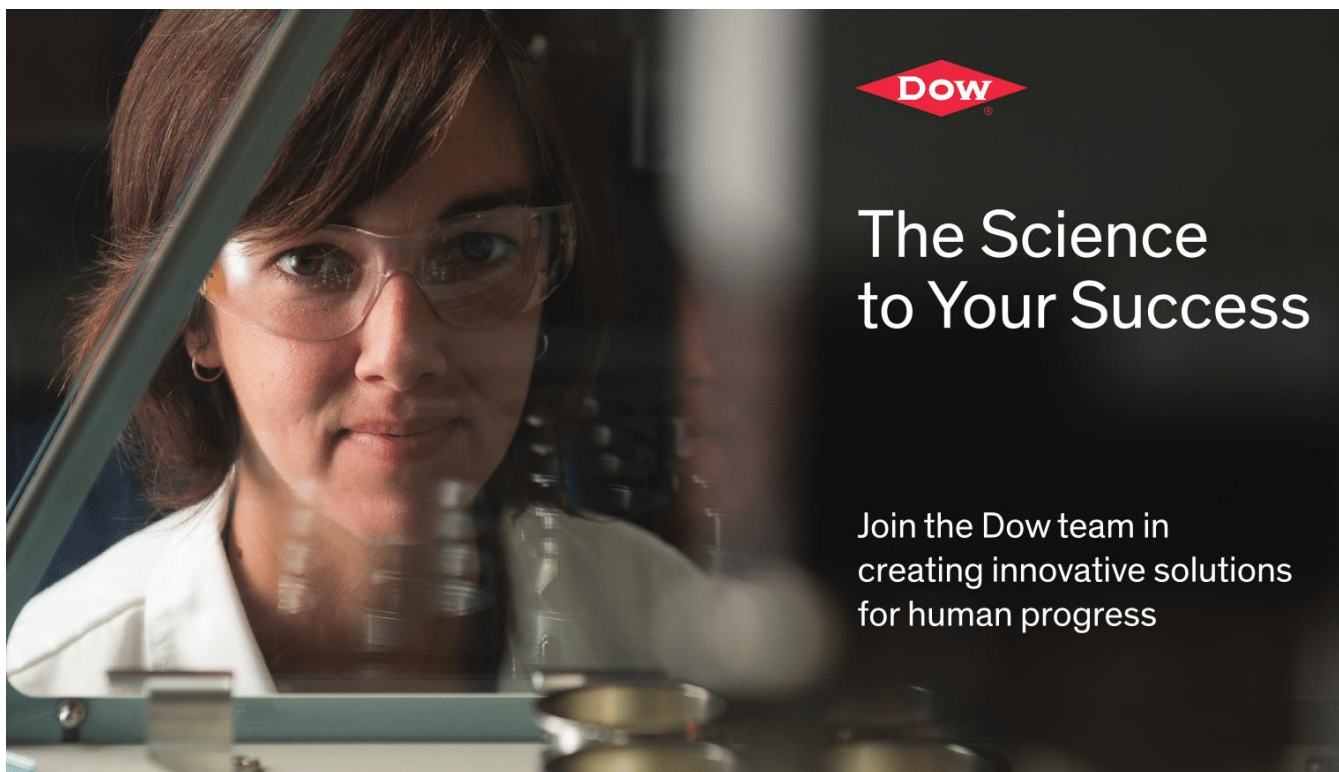


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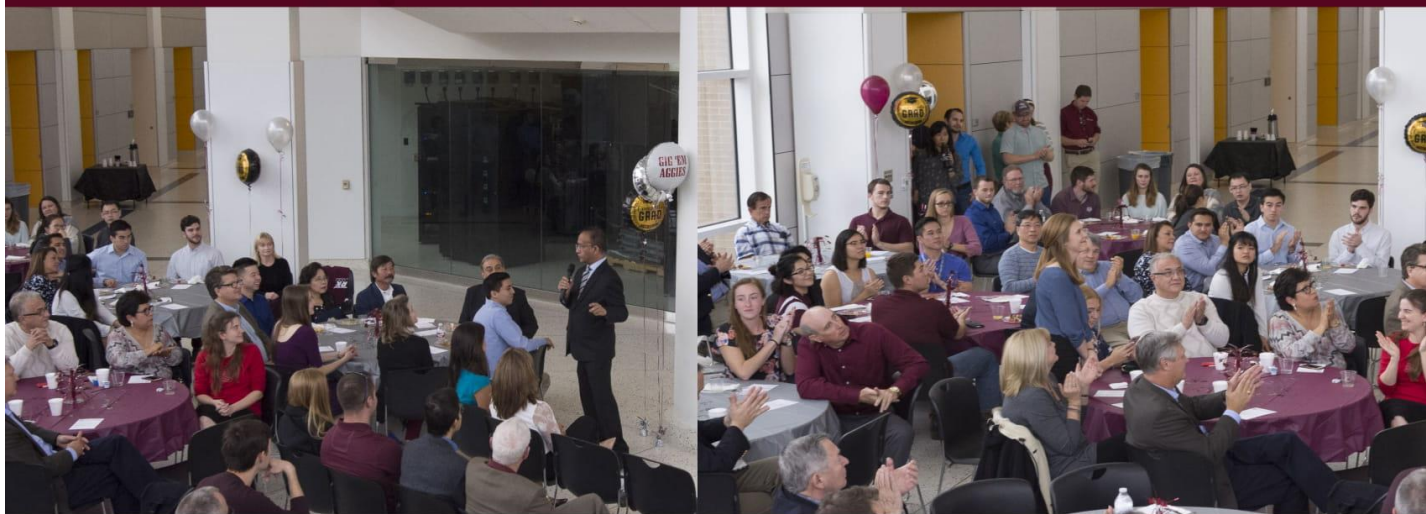
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The Artie McFerrin Department of Chemical Engineering is one of the top rated chemical engineering departments in the world. It is also one of the largest, fully accredited chemical engineering programs in the country. The department has become a prolific 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          |

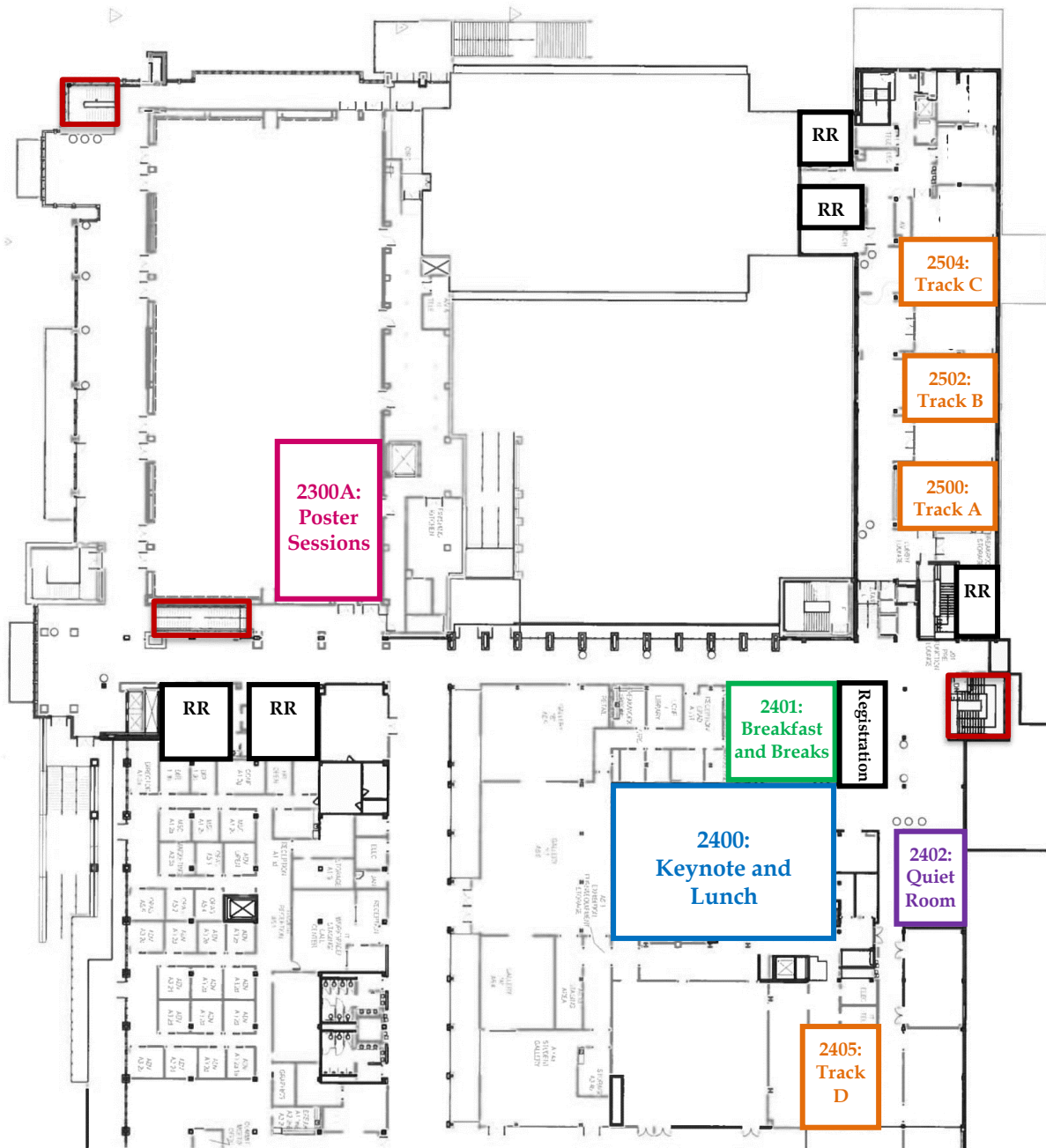
## Faculty

|                               |           |
|-------------------------------|-----------|
| <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**