

# **The 57<sup>th</sup> ACS DFW Meeting-in-Miniature**

**at**

**East Texas A&M University  
Commerce, TX**

**April 26, 2025**





# EAST TEXAS A&M

## MAIN CAMPUS

**Driving**  
 The Welcome Center ★  
 2104 University Dr.  
 Commerce, TX 75428

**Mailing Envelopes**  
 P.O. Box 3011  
 Commerce, Texas 75429

**Shipping Packages**  
 2600 South Neal St.  
 Commerce, TX 75428

**Undergraduate Admissions**  
 903.886.5000

**Graduate Admissions**  
 903.886.5163

Explore campus through our interactive map at [tamuc.edu/map](http://tamuc.edu/map).



## BUILDINGS

D3 Agriculture, Engineering & Technology, Austin (AG/ET)  
 D5 Alumni Center  
 D2 Art (ART)  
 B3 Art Sculpture Lab (ASL)  
 C7 Binnion Hall (BIN)  
 B5 Education North, Young  
 C4 Education South, Sowers  
 F3 Employee Services  
 C5 Ferguson Auditorium and Social Sciences (SS)

A3 Field House (FH)  
 A2 Football Locker Room  
 B4 Halladay Student Services  
 B6 Health Services  
 B6 Henderson Hall (HEN)  
 D6 Heritage House/Lyday Gardens  
 D7 Journalism (JOUR)  
 C1 Lakeside Pavilion  
 C3 Library, Velma K. Waters  
 C2 McDowell Administration (BA)  
 A1 Memorial Stadium

F1 Morris Recreation Center (MRC)  
 B2 Music (MUS)  
 F2 New Pride Apartments  
 E1 Nursing and Health Sciences  
 D1 Performing Arts Center (PAC)  
 H2 Phase II Residence Hall  
 G1 Phase III Residence Hall  
 E2 Planetarium  
 B6 Police  
 B3 Postal Services  
 A5 Prairie Crossing Residence Hall

H1 Pride Rock Residence Hall  
 E3 Rayburn Student Center (RSC)  
 E2 Science, McFarland (STC)  
 C6 Sororities & Women's Halls  
 D8 Talbot Hall of Languages (DTH)  
 D4 Wathena Temple Fine Arts (WTFA)  
 B1 Welcome Center ★  
 A4 Whitley Gymnasium  
 H3 Whitley Residence Hall



## **Program outline**

**Check-in 8:30am –**

Coffee break, 10:30 - 11 am

Session 1 Physical I, 9:00 am - 12 pm (room #127)

Session 2 Chemical Education, 9:00 am - 12 pm (room 146)

Session 3 Undergraduate I, 9:30 am - 12 pm (room # 135)

Session 4 Analytical I, 9:30 am - 12 pm (room #122)

Session 5 Biochemistry, 9:30 - 11:30 am (room #107)

Session 6 Inorganic, 9:30am - 12 pm (room #123)

**Lunch 12-1pm (at the Cafeteria of Student Center,  
lunch hour: 11am to 3pm)**

Coffee break, 2 - 2:15 pm

Session 7 Physical II, 1- 3:45 pm (room #127)

Session 8 Undergraduate II, 1 – 2:45 pm (room # 135)

Session 9 Analytical II, 1 - 2:45 pm (room #122)

Session 10 Organic, 1 - 2:45 pm (room #107)

Session 11 Material, 1 – 3:30 pm (room #123)

**Award Ceremony (room #127), 4:00pm-**

**Session 1: Physical I  
Room 127**

**Chair: TBA  
Judge: TBA**

- P1 9:00 AM Presenter: Afifa Yousaf Southern Methodist University  
Signatures of Hydrogen Bonding in Soft X-ray Spectroscopy
- P2 9:15 AM Presenter: Sarthi Polara  
Computational Investigation of the Inhibition Mechanism of DNA Polymerase Lambda by Cytarabine
- P3 9:30 AM Presenter: Jaya Pathak University of North Texas  
Investigating the Effect of Force Fields and Water Models on Unbinding Kinetics of the SH3-SOS (Protein-Peptide) Complex using Atomistic Simulations
- P4 9:45 AM Presenter: Dipesh Shrestha University of North Texas  
Unraveling the Dissociation Kinetics of Barnase-Barstar Complex in Full Atomistic Detail
- P5 10:00 AM Presenter: Kriti Alam University of North Texas  
Classifying Molecular Crystal Polymorphs using SOAP-PCA
- P6 10:15 AM Presenter: Upeksha C. Dissanayake University of Texas at Dallas  
Computational Characterization of the Impact of Cancer Associated Mutations on DNA Glycosylase Enzyme Structure and Dynamics
- 10:30 AM Break
- P7 11:00 AM Presenter: Alexis Ann Delgado Southern Methodist University  
Hybrid and Mixed Basis Set Strategies for XPS Calculations of Small Water Clusters
- P8 11:15 AM Presenter: Aloka Senanayaka University of North Texas  
Unraveling the Effect of Force Fields and Salt Concentration on the Dissociation Kinetics of MDM2-p53 Protein-Peptide Complex Via Infrequent Meta-Dynamics Simulations
- P9 11:30 AM Presenter: Daniel Devore Southern Methodist University  
Pursuing rank reduced CCSD(T) for open-shell systems
- P10 11:45 AM Presenter: Duc Lai Southern Methodist University  
The Electric Field-perturbed Potential Energy Surface

12:00 noon Lunch break

**Session 2: Chemical Education  
Room 146**

**Chair: TBA  
Judge: TBA**

CE 1      9:00 AM      Presenter: Mark Bertolami      University of North Texas  
Embracing Cognitive Diversity: Neurodivergent Chemistry Majors' Lecture Experiences Across the Chemistry Curriculum

CE 2      9:15 AM      Presenter: Cristina Castillo      University of North Texas  
Student Experiences and Faculty Perceptions of Chemistry Graduate Education: A National Study

CE 3      9:30 AM      Presenter: Donald Charles Ballew      University of North Texas  
Working Title - Teaching FTIR and Raman in Undergraduate Laboratories

CE 4      9:45 AM      Presenter: Haiyan Alfulaiti      University of North Texas  
Exploring Students' Understanding of Atomic Spectra: A Construct Modeling Approach

CE 5      10:00 AM      Presenter: Jessie Stenlund      University of North Texas  
Evaluating the Impact of a Guided-Inquiry Liquid-Liquid Extraction Experiment on Student Learning and Confidence

CE 6      10:15 AM      Presenter: Olajumoke Mary Ayeni      University of North Texas  
Extraction Strategies for Problem Solving in the Context of VSEPR Theory

10:30 AM      Break

CE 7      11:00 AM      Presenter: Matthew Breuer      University of North Texas  
Eliciting Organic Chemistry Students' Epistemological Beliefs by a Novel Method

CE 8      11:15 AM      Presenter: Nicholette Stewart      University of North Texas  
Addressing Key Contributors to Burnout in Chemistry Graduate Education

CE 9      11:30 AM      Presenter: Sophie Ntipouna      University of North Texas  
Investigating the Epistemic Affect in Scientific Learning: A Dynamic Approach using Affective MDMs

CE 10      11:45 AM      Presenter: Mary Tess Urbanek      University of North Texas  
It Makes Me Feel Better... Just Because They Said I Had a Solid Argument:" Characterization of Student Interaction with Peer Feedback

12:00 noon      Lunch break

**Session 3: Undergraduate I  
Room 135**

**Chair: TBA  
Judge: TBA**

UG 01      9:30 AM      Presenter: Trang Nguyen      University of Texas at Dallas

The Atmospheric Chemistry of Fluoroacetonitrile and the Characterization of the Major Product, Cynoformyl Fluoride

UG 02      9:45 AM      Presenter: Daillin Perez      University of North Texas

Structural Analysis of Synthetic Opioids using Travelling Wave Ion Mobility-Mass Spectrometry (TWIM-MS)

UG 03      10:00 AM      Presenter: Aman Rahman      University of Texas at Dallas  
Enhanced Metal-Organic Framework Polymer Composites for Hazardous Chemical Absorption

UG 04      10:15 AM      Presenter: Evan Soward

Osajin Effectively Kills Pancreatic Tumor Cells but Exhibits Very Little Toxicity to Normal Cells

10:30 AM      Break

UG 05      11:00 AM      Presenter: Debby Sunday      University of Texas at Arlington  
Natural product extracts as photosensitizers for the photodynamic inactivation of bacteria

UG 06      11:15 AM      Presenter: William Connor Nelson      Texas Wesleyan University  
Utilizing <sup>1</sup>H-NMR to Determine Protonation State in Oral Nicotine Pouches

UG 07      11:30 AM      Presenter: Daniel Pearson      University of Texas at Arlington  
Computational Characterization of Hafnium-Based Polymers and Cross-Linking Behavior

UG 08      11:45 AM      Presenter: Phat Dinh      University of Texas at Arlington  
Optimization of Polyethyleneimine Functionalized Spongy Monoliths for Lipid Nanoparticle Separations using Liquid Chromatography-Mass Spectrometry

12:00 noon      Lunch break

**Session 4: Analytical I  
Room 122**

**Chair: TBA  
Judge: TBA**

A 01      9:30 AM      Presenter: Piumi Poornima Kularathne      University of North Texas  
Selenium Vacancy Rich Exfoliated Molybdenum Selenide for Highly Efficient Electro Catalytic Nitrate  
Reduction to Ammonia

A 02      9:45 AM      Presenter: Richard McCrary      University of North Texas  
Analysis of Fragmentation Patterns and Pathways for Fentanyl Analogues Obtained by APCI-GC-MS

A 03      10:00 AM      Presenter: Chamari Vijanga Ileperuma      University of North Texas  
Phenothiazine-C60 Based Multi-Modular Donor-Acceptor Systems Highlighting the Exceptional  
Electron Accepting Properties of C60 in Strong Acceptor Integrated Conjugates

A 04      10:15 AM      Presenter: Alankar Kafle      University of North Texas  
Enhancing the Electrocatalytic Dinitrogen Reduction Reaction with Selenium Vacancy in Transition  
Metal Dichalcogenides

10:30 AM      Break

A 05      11:00 AM      Presenter: Chelsi Wilson      University of North Texas  
Development of Abraham Model Correlations for Predicting the Solubility of Crystalline Organic  
Compounds and Inorganic Gases in Ethyl Formate

A 06      11:15 AM      Presenter: Chimauchem Valentine Odinaka      University of Texas-Arlington  
Edman Sequencing Evolved: Precise Native Peptide C-Terminal Ligation

A 07      11:30 AM      Presenter: Andrew Dawson      University of North Texas  
Understanding the Role of Donor-Tetracyanobutadiene on Porphyrin Beta-Periphery Towards Ultrafast  
Charge Transfer Dynamics

A 08      11:45 AM      Presenter: Joisha Girme      University of Texas at Arlington  
Rapid Inexpensive Measurement of Urinary Iodide

12:00 noon      Lunch break

**Session 5: Biochemistry  
Room 107**

**Chair: TBA  
Judge: TBA**

B 01      9:30 AM      Presenter: Cary Darwin      University of Texas at Dallas  
Enhancing viral insight: A user-friendly website for the customized modification of viruses and virus-like particles for visualization

B 02      9:45 AM      Presenter: Debdatta Das      University of Texas at Arlington  
Development of a pH-responsive peptide-based hydrogel for effective eradication of MRSA biofilm

B 03      10:00 AM      Presenter: Emmanuel Brefo      East Texas A&M University  
Effect of Pyrimidine Supplementation on Pullulan Production by *Aureobasidium pullulans* ATCC 201253

B 04      10:00 AM      Presenter: Francis N. Eze      University of North Texas  
Structure Activity Relationship Studies of Triazole-Based Factor XIIa Inhibitors.

B 05      10:15 AM      Presenter: Juliana Dias      University of Texas at Dallas  
Histone variant H2A.Z enhances histone and nucleosome dynamics

10:30 AM      Break

B 06      11:00 AM      Presenter: Gurleen Kaur      University of Texas at Arlington  
Investigation of photoactive metallodrugs as antimicrobials

B 07      11:15 AM      Presenter: Trang Nguyen      University of Texas at Dallas  
Understanding the Role of Histone Chaperone RBBP4 in Regulating Chromatin Structure

B 08      11:30 AM      Presenter: Caylie Casto      Southern Methodist University  
Blue Light Receptor 1: Homologs, Interactions, and its Role in Fungal Systems and Beyond

12:00 noon      Lunch break

**Session 6: Inorganic  
Room 123**

**Chair: TBA  
Judge: TBA**

I 01      9:30 AM    Presenter: Achala Gamarallage    University of Texas at Arlington  
Sterically Hindered Pyridyl-Based Coinage Metal Complexes

I 02      9:45 AM    Presenter: Alisher Talgatov    University of Texas at Arlington  
Applications of Photoactivated Metallodrugs for Cancer Therapy

I 03      10:00 AM    Presenter: Arefeh Mirsharifian    University of Texas at Dallas  
Removal of Per- and Polyfluoroalkyl Substances from Contaminated Groundwater Using Cationic Metal–Organic Frameworks

I 04      10:15 AM    Presenter: Bita Amiri    University of Texas at Arlington  
Sustainable Pigments Made by Applying Chemical Pressure on 2D Rosiaite-based structures

10:30 AM    Break

I 05      11:00 AM    Presenter: Dalton Lucas    University of Texas at Arlington  
Synthesis and Characterization of Light-Triggered Metal Complexes for Cancer Treatment

I 06      11:15 AM    Presenter: Deepika Virendra Karade    University of Texas at Arlington  
Probing the Influence of Phenanthroline-Based Ligands on Group 11 Metal-ethylene Complexes: Discoveries and Catalytic Prospects

I 07      11:30 AM    Presenter: Olajumoke Mary Ayeni    University of North Texas  
Superhydrophobic Methylated Metal–Organic Frameworks (MeMOFs) for Water Purification and Oil Extraction

I 08      11:45 AM    Presenter: Vo Phan    University of Texas at Arlington  
Exploring Copper(I) -Cyclopropene Complexes

12:00 noon    Lunch break

**Session 7: Physical II  
Room 127**

**Chair: TBA  
Judge: TBA**

P 11 1:00 PM Presenter: Fernando Montalvillo Ortega University of Texas at Dallas  
Microsecond-Scale Electrophysiology Simulations of Unconventional Ion transporter Fluc

P 12 1:15 PM Presenter: Logan Estridge University of North Texas  
Understanding the Molecular Crystal Polymorphism of p-Aminobenzoic Acid via Machine Learning Potentials

P 13 1:30 PM Presenter: M. N. Hasna Begam University of Texas at Dallas  
A Coarse-Grained Computational Model for Investigating Drug Release Mechanisms in Azobenzene-Derivatized Liposomes

P 14 1:45 PM Presenter: Noah Smith East Texas A&M University  
Hydrochars Derived from Contaminated Chlorella for Biosorption of Heavy Metals in Wastewater

Coffee break 2:00 PM - 2:15 PM

P 15 2:15 PM Presenter: Pradip Si University of North Texas  
Molecular Dynamic Simulation of ROY Polymorphic Crystals

P 16 2:30 PM Presenter: Savi Savi University of North Texas  
Kinetics of halogenated compounds with atmospheric radicals

P 17 2:45 PM Presenter: Shamberia Thomas Texas Christian University  
Yield of protein crystallization from metastable liquid-liquid phase separation

P 18 3:00 PM Presenter: Shikshya Bhusal University of North Texas  
Impact of Different Binding Orientations of linker on PROTAC Conformations: A Computational comparative Study of dBET6 and dBET23

P 19 3:15 PM Presenter: Shubham Chatterjee University of Texas at Dallas  
Impact of a Cancer-Associated Mutation on Poly (ADP-ribose) Polymerase I Inhibition

P 20 3:30 PM Presenter: Oriana Silva University of North Texas  
Investigating the Dissociation Mechanisms of 14-3-3/PMA2 Protein Complexes in the Presence of Stabilizing Molecules via Atomistic Simulations

**Session 8 : Undergraduate II  
Room 135**

**Chair: TBA  
Judge: TBA**

UG 09      1:00 PM      Presenter: Grant Vavro      University of Texas at Dallas  
Synthesis of a Novel 2D Lead-Halide Perovskite for Understanding Structure Property Relationships

UG 10      1:15 PM      Presenter: Pavan Ahluwalia      University of North Texas  
Anticorrosive Strategies for Cu-Al Wire-Bonded Devices in Extreme Automotive Applications

UG 11      1:30 PM      Presenter: Esteban Rodriguez      Hardin-Simmons University  
Synthesis and Characterization of a Ferrocene-Thymol Derivative

UG 12      1:45 PM      Presenter: Kilee Lasiter      East Texas A&M University  
Kinetic and Isotherm Analysis of Heavy Metal Biosorption using *Chlorella Pyrenoidosa* in Waste Water

Coffee break 2:00 PM - 2:15 PM

UG 13      2:15 PM      Presenter: Jenny Ngan Nguyen      University of Texas at Arlington  
Design and Synthesis of Self-Assembling Peptides for Hydrogel Formation

UG 14      2:30 PM      Presenter: Theodore Nguyen      University of Dallas  
Jet Fuel Bioremediation via Terminal Oxidation of n-alkanes by *Pseudomonas aeruginosa*

**Session 9: Analytical II  
Room 122**

**Chair: TBA  
Judge: TBA**

A 09          1:00 PM          Presenter: Kamal Dhakal    University of North Texas

Porphyrin Based Conductive Polymer Derived from Tetrakis [biphenyl bis (bithiophene)] Porphyrinato Cobalt (II) for Efficient Electrochemical Nitrate Reduction to Ammonia

A 10          1:15 PM          Presenter: Manan Guragain    University of North Texas

Photo-enhanced Electrochemical Conversion of Nitrate to Ammonia Via Sulfur Vacancy-Rich Exfoliated MoS<sub>2</sub>

A 11          1:30 PM          Presenter: Michael Bawuah Owusu    East Texas A&M University  
Effect of the His, Cys, or Asp substituent groups on the gas- and solution- phase zinc affinities of the Acetyl-Aa1-Aa2-Gly3-Pro4-Tyr5-His6-Cys7 heptapeptides and comparison with the His-tag

A 12          1:45 PM          Presenter: MK Altafi    University of North Texas

Electrochemical Reduction of Nitrate to Ammonia at Oxidized Vanadium Surfaces with V (3+) and V (4+) Oxidation States.

Coffee break 2:00 PM - 2:15 PM

A 13          2:15 PM          Presenter: Ram Ratan Kaswan    University of North Texas

Intervalence Charge Transfer, and Exothermic and Isoenergetic Symmetry Breaking Charge Separation in Far-Red Capturing Zinc Phthalocyanine Dimers

A 14          2:30 PM          Presenter: Richmond Amankwaah Adomako    East Texas A&M University

Characterization of Zinc-Binding Heptapeptides as a Replacement for the His Tag in Improved Protein Purification Efficiency

**Session 10: Organic  
Room 107**

**Chair: TBA  
Judge: TBA**

O 01      1:00 PM      Presenter: Calvin Heyl      University of Texas at Arlington  
Development of Chemoselective Reactions for Amino Acid Sidechains

O 02      1:15 PM      Presenter: Aisosa Omere      University of Texas at Arlington  
Edman Sequencing Evolved: Precise Native Peptide C-Terminal Ligation

O 03      1:30 PM      Presenter: Desiree Czapski      University of Texas at Arlington  
Bioorthogonal Engineering of Trehalose-Modified Glycolipids in Mycobacterium: Unraveling  
Molecular Interactions via Click Chemistry

O 04      1:45 PM      Presenter: Hansani S. A. Amarasuriyage      University of Texas at Dallas  
Investigation of Viscoelastic Properties of Poly(3-hexylthiophene)-b-poly (n-butyl acrylate) Diblock  
Copolymers Using Linear Viscoelastic Nanoindentation Technique

Coffee break 2:00 PM - 2:15 PM

O 05      2:15 PM      Presenter: Marius Popa      University of Texas at Dallas  
Novel Pyrrole-Based Donor-Acceptor Dyes for Organocatalyzed Atom Transfer Radical Polymerization  
(O-ATRP)

O 06      2:30 PM      Presenter: Stanley Dugbartey      East Texas A&M University  
Recognition of Perfluoroalkyl Substances via a Synthetic Porphyrin Compound

**Session 11: Material  
Room 123**

**Chair: TBA  
Judge: TBA**

M 01      1:00 PM      Presenter: Hoa Nguyen      University of Texas Arlington  
Covalency and Lone Pair Driven Distortions in Sulfur Doped Tin Niobate Pigments

M 02      1:15 PM      Presenter: Ariel Tolfree      University of Texas at Dallas  
Mechanoresponsive Polymers for Damage/Defect Detection in 3D Printing

M 03      1:30 PM      Presenter: Emily E. Osborn      University of Texas at Dallas  
MOFylation: The Encapsulation and Preservation of Microorganisms Using ZIF-8

M 04      1:45 PM      Presenter: Lida Aeindartehr      Southern Methodist University  
Polymorph Studies of Ethosuximide and Its Co-Crystal Formation with Lamotrigine

Coffee break 2:00 PM - 2:15 PM

M 05      2:15 PM      Presenter: Lyndsay Ayers      University of Texas at Dallas  
The Effects of Chitosan Source on the Properties of 3D Printed Polymer Composites

M 06      2:30 PM      Presenter: Miguel Gaspar      University of Texas at Dallas  
Hybrid Organic Molecular Crystal Assembly as a Thermo-Controlled Artificial Muscle

M 07      2:45 PM      Presenter: Noreen Mazhar      University of Texas at Dallas  
Covalent Organic Frameworks: A 2D Platform for Controlled Nano Structuring of Single Ion Magnets

M 08      3:00 PM      Presenter: Stella Amagbor      University of North Texas  
Impact of Surface Oxidation on Catalytic Activity in CO Hydrogenation over MoxC Thin Films  
Deposited at Different Temperatures

M 09      3:15 PM      Presenter: Md Tareque Hassan Mukut      University of Texas at Arlington  
Design, Characterization, and Bioassay of Zwitterionic Antimicrobial Polymers for Biofilm Modulation:  
A Cu-Catalyzed Click Chemistry Approach