

The 57th 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.



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:
Judge:**

**TBA
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 ¹H-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 Viyanga 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) Polymerase1 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 MoS₂

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:
Judge:**

**TBA
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