

The 57th ACS DFW Meeting-in-Miniature

at

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

April 26, 2025



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- 4 pm (room #127)

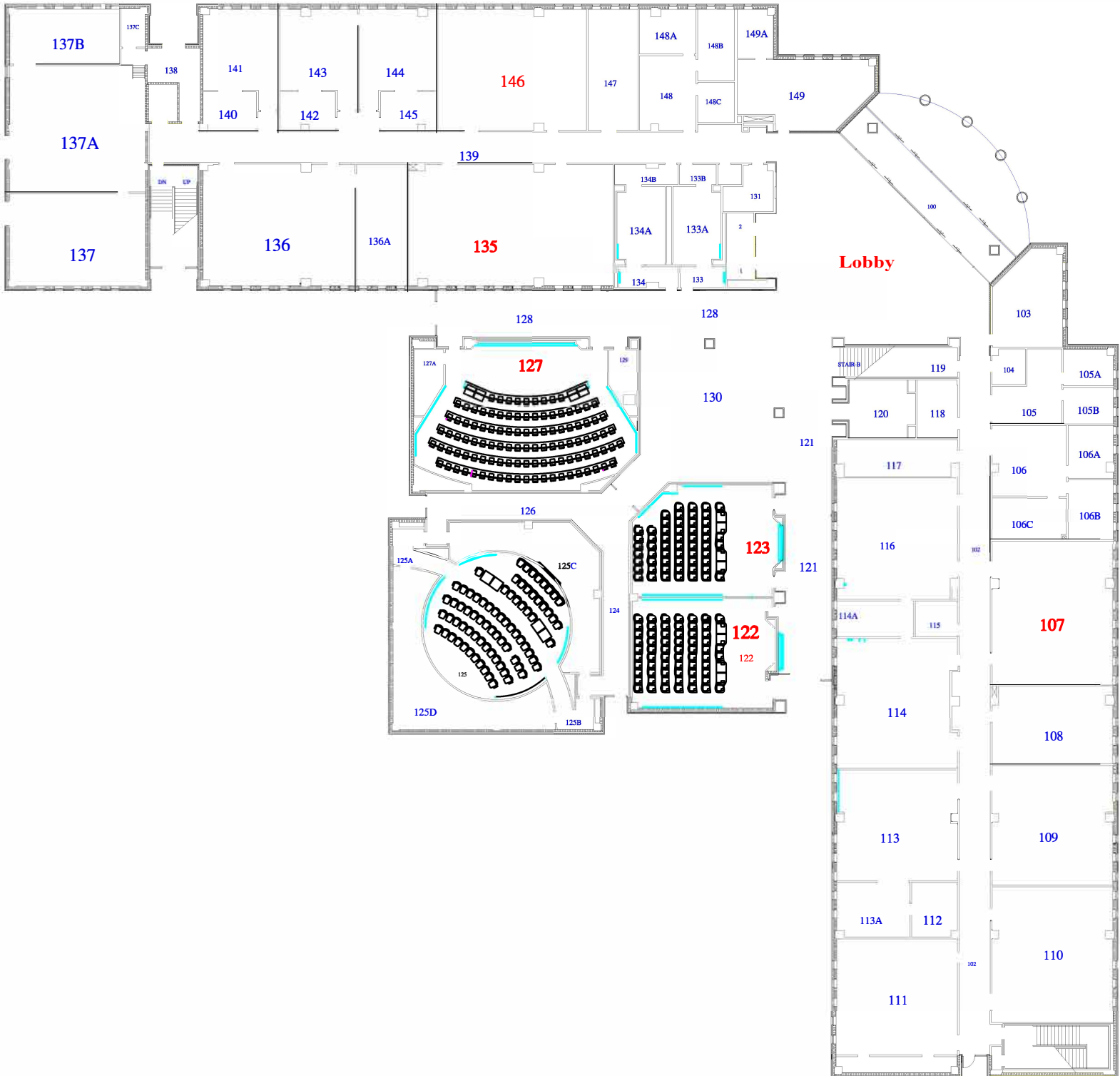
Session 8 Undergraduate II, 1 - 3 pm (room # 135)

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

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

Session 11 Material, 1 - 4 pm (room #123)

Award Ceremony (room #127), 4:30pm-



McFarland Science Building
 Building Number 0699
 First Floor

East Texas A&M University
 109,463 Gross Square Feet
 41,428 Gross Square Feet First Floor
 [1,152]-Foot Perimeter
 Scale 1/8" = 1'-0"

North
 Constructed 2006
 Revised 10/15/2019 cns

**Session 1: Physical I
Room 127**

**Chair:
Judge:**

**TBA
TBA**

P1 9:00 AM Presenter: Afifa Yousaf
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
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
Unraveling the Dissociation Kinetics of Barnase-Barstar Complex in Full Atomistic Detail

P5 10:00 AM Presenter: Kriti Alam
Classifying Molecular Crystal Polymorphs using SOAP-PCA

P6 10:15 AM Presenter: Upeksha C. Dissanayake
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 Antoinette Ann Delgado
HYBRID AND MIXED BASIS SET STRATEGIES FOR XPS CALCULATIONS OF SMALL WATER
CLUSTERS

P8 11:15 AM Presenter: Aloka Senanayaka
Unraveling the Effect of Force Fields and Salt Concentration on the Dissociation Kinetics of MDM2-
p53 Protein-Peptide Complex Via Infrequent Metadynamics Simulations

P9 11:30 AM Presenter: Daniel Devore
Pursuing rank reduced CCSD(T) for open-shell systems

P10 11:45 AM Presenter: Duc Lai
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
Embracing Cognitive Diversity: Neurodivergent Chemistry Majors' Lecture Experiences Across the Chemistry Curriculum

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

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

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

CE 5 10:00 AM Presenter: Jessie Stenlund
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
Extraction Strategies for Problem Solving in the Context of VSEPR Theory

10:30 AM Break

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

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

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

CE 10 11:45 AM Presenter: Mary Tess Urbanek
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

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

UG 02 9:45 AM Presenter: Daillin Perez

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

UG 03 10:00 AM Presenter: Aman Rahman

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

Natural product extracts as photosensitizers for the photodynamic inactivation of bacteria

UG 06 11:15 AM Presenter: William Connor Nelson

Utilizing ¹H-NMR to Determine Protonation State in Oral Nicotine Pouches

UG 07 11:30 AM Presenter: Daniel Pearson

Computational Characterization of Hafnium-Based Polymers and Cross-Linking Behavior

UG 08 11:45 AM Presenter: Phat Dinh

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
Selenium Vacancy Rich Exfoliated Molybdenum Selenide for Highly Efficient Electro catalytic Nitrate Reduction to Ammonia

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

A 03 10:00 AM Presenter: Chamari Vijanga Ileperuma
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
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
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 Odinka
Edman Sequencing Evolved: Precise Native Peptide C-Terminal Ligation

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

A 08 11:45 AM Presenter: Joisha Girme
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

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

Development of a pH-responsive peptide-based hydrogel for effective eradication of MRSA biofilm

B 03 10:00 AM Presenter: Emmanuel Brefo

Effect of Pyrimidine Supplementation on Pullulan Production by *Aureobasidium pullulans* ATCC 201253

B 04 10:00 AM Presenter: Francis N. Eze

Structure Activity Relationship Studies of Triazole-Based Factor XIIa Inhibitors.

B 05 10:15 AM Presenter: Juliana Dias

Histone variant H2A.Z enhances histone and nucleosome dynamics

10:30 AM Break

B 06 11:00 AM Presenter: Gurleen Kaur

Investigation of photoactive metallodrugs as antimicrobials

B 07 11:15 AM Presenter: Trang Nguyen

Understanding the role of histone chaperone RBBP4 in regulating chromatin structure

B 08 11:30 AM Presenter: Caylie Casto

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 Wagure Gamarallage
Sterically Hindered Pyridyl-Based Coinage Metal Complexes

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

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

I 04 10:15 AM Presenter: Bitu Amiri
Sustainable Pigments Made by Applying Chemical Pressure on 2D Rosiaite-based structures

10:30 AM Break

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

I 06 11:15 AM Presenter: Deepika Virendra Karade
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
Superhydrophobic Methylated Metal-Organic Frameworks (MeMOFs) for Water Purification and Oil Extraction

I 08 11:45 AM Presenter: Vo Phan
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
Microsecond-scale electrophysiology simulations of unconventional ion transporter Fluc

P 12 1:15 PM Presenter: Kriti Alam
Classifying Molecular Crystal Polymorphs using SOAP-PCA

P 13 1:30 PM Presenter: Logan Estridge
Understanding the Molecular Crystal Polymorphism of p-Aminobenzoic Acid via Machine Learning Potentials

P 14 1:45 PM Presenter: M. N. Hasna Begam
A Coarse-Grained Computational Model for Investigating Drug Release Mechanisms in Azobenzene-Derivatized Liposomes

Coffee break 2:00 PM - 2:15 PM

P 15 2:15 PM Presenter: Noah Smith
Hydrochars Derived from Contaminated Chlorella for Biosorption of Heavy Metals in Wastewater

P 16 2:30 PM Presenter: Pradip Si
Molecular Dynamic Simulation of ROY Polymorphic Crystals

P 17 2:45 PM Presenter: Savi Savi
Kinetics of halogenated compounds with atmospheric radicals

P 18 3:00 PM Presenter: Shamberia Thomas
Yield of protein crystallization from metastable liquid-liquid phase separation

P 19 3:15 PM Presenter: Shikshya Bhusal
Impact of Different Binding Orientations of linker on PROTAC Conformations: A Computational comparative Study of dBET6 and dBET23

P 20 3:30 PM Presenter: Shubham Chatterjee
Impact of a Cancer-Associated Mutation on Poly(ADP-ribose) Polymerase1 Inhibition

P 21 3:45 PM Presenter: Oriana Silva
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
Synthesis of a Novel 2D Lead-Halide Perovskite for Understanding Structure Property Relationships

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

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

UG 12 1:45 PM Presenter: Claudia Claridy
Characterizing the Interaction between RBBP4 and Histones H3-H4

Coffee break 2:00 PM - 2:15 PM

UG 13 2:15 PM Presenter: Kilee Lasiter
Kinetic and isotherm analysis of heavy metal biosorption using *Chlorella pyrenoidosa* in wastewater

UG 14 2:30 PM Presenter: Jenny Ngan Nguyen
Design and Synthesis of Self-Assembling Peptides for Hydrogel Formation

UG 15 2:45 PM Presenter: Theodore Nguyen
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

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

Photo-enhanced Electrochemical Conversion of Nitrate to Ammonia Via Sulfur Vacancy-Rich Exfoliated MoS₂

A 11 1:30 PM Presenter: Michael Bawuah Owusu

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

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

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

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
Development of Chemoselective Reactions for Amino Acid Sidechains

O 02 1:15 PM Presenter: Aisosa Omere
Edman Sequencing Evolved: Precise Native Peptide C-Terminal Ligation

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

O 04 1:45 PM Presenter: Hansani S. A. Amarasuriyage
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
Novel Pyrrole-Based Donor-Acceptor Dyes for Organocatalyzed Atom Transfer Radical Polymerization (O-ATRP)

O 06 2:30 PM Presenter: Stanley Dugbartey
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
Covalency and Lone Pair Driven Distortions in Sulfur Doped Tin Niobate Pigments

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

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

M 04 1:45 PM Presenter: Lida Aeindartehr
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
The Effects of Chitosan Source on the Properties of 3D Printed Polymer Composites

M 06 2:30 PM Presenter: Maryam Piroozzadeh
Cationic Covalent Organic Framework as Fluorescent Sensor for the Detection of Poly- and Perfluoroalkyl Substances (PFAS)

M 07 2:45 PM Presenter: Miguel Gaspar
Hybrid Organic Molecular Crystal Assembly as a Thermo-Controlled Artificial Muscle

M 08 3:00 PM Presenter: Nafees Iqbal
Cationic Covalent-Organic Frameworks (COFs): A Sensing Probe for the Detection of Per- and Polyfluorinated Substances (PFAS)

M 09 3:15 PM Presenter: Noreen Nguyen
Covalent Organic Frameworks: A 2D Platform for Controlled Nanostructuring of Single Ion Magnets

M 10 3:30 PM Presenter: Stella Amagbor
Impact of surface oxidation on catalytic activity in CO hydrogenation over MoxC thin films deposited at different temperatures

M 11 3:45 PM Presenter: Md Tareque Hassan Mukut
Design, Characterization, and Bioassay of Zwitterionic Antimicrobial Polymers for Biofilm Modulation: A Cu-Catalyzed Click Chemistry Approach