



SWRM2023

chemistry energized

Southwest Regional Meeting



ACS

Chemistry for Life™

Nov 15-18, 2023 • Omni Hotel • Oklahoma City, OK

Preliminary .PDF Program*



SWRM.org

On-line Meeting app
(<https://bit.ly/swrm-2023>)



This document is up to date as of November 13, 2023. An up-to-date program will be on the on-line app above.

*Note: This pdf is for the convenience of participants. At the meeting, you will see references around the meeting halls that will be linked to the most recent version of the meeting program. Changes in the assignments/events in this document are possible. Please refer to the SWRM23 Meeting app for current information. That app should be the authoritative source as of the week of the meeting.

Special Event Lectures

Wednesday, November 15, 2023

4:45 - 5:30 PM



Prof. Karen Wooley

Distinguished Professor of Chemistry, Texas A&M University

Sustainable Plastics from Sugar

Oklahoma Station 6



Dr. James Seaba

Program Director, ARPA-E

**GREENWELLS, Grid-free Renewable Energy Enabling
New Ways to Economical Liquids and Long-term Storage**

Oklahoma Station 1



Hon. Jacob Rosecrants

Oklahoma House of Representatives

Oklahoma House of Representatives Current Activities

Oklahoma Station 3

Thursday, November 16, 2023

4:45 - 5:30 PM



Dr. Bill Carroll

Retired, OxyChem

**Vinyl Chloride, Cancer and Technology:
How Science Saved a Business**

Oklahoma Station 2



Prof. Kayunta Johnson-Winters

Associate Professor, University of Texas-Arlington

Diversity in Chemistry

Oklahoma Station 2



Prof. Angela Gronenborn

Rosalind Franklin Professor and Chair, University of Pittsburgh
School of Medicine

**The Art of Border Crossings –
Integrative Multidisciplinarity in the Natural Sciences**

Myriad

Special Presentation

Thursday, November 16, 2023

10:00 AM



A special presentation will be given in honor of the life and professional career of Professor Allen Apblett, colleague and long-time Councilor from the Oklahoma Section of the ACS.

Best Practices for Successful Small Chemical Businesses

Omni Oklahoma City Hotel, Bricktown

10:00 307 The creation of lasting successful chemical businesses in Oklahoma, the legacy of Dr. Allen Apblett. **N.F. Materer**

Contact

General Information

Cheryl Frech (cfrech@uco.edu) and Lloyd Bumm (bumm@ou.edu)

Program Information

Please see SWRM2023.org or contact Frank Blum (fblum@okstate.edu) or Elijah Schnitzler (elijah.schnitzler@okstate.edu)

Exhibition Opportunities (Commercial or Academic)

Please see SWRM2023.org or contact Charles Rice (expo@swrm2023.org)

Meeting Schedule by Track

Scroll to see events for Energy, Materials, Organic/Medicinal, Biological, Education, Special Event Lectures, Special Symposia, General (Continuing) Workshops, Meal and Social Events

Key: A = AM, P = PM, D = AM & PM, E = Evening, B = Breakfast, L = Lunch

Energy Track

Symposium	W	Th	F	Sa
Hydrocarbons: Exploration, Development, Refining and Processing - Oral	A			
" Posters	P			
Chemical Production at Industrial Scale - Oral		D		
Sustainability and Environmental Issues in Hydrocarbon Production - Oral			A	
" Posters		P		
Solar, Fuel, Wind and Future Energy	P	A		
" Posters		P		
Catalysis and Energy: Inextricable Links in the Chain of Progress - Oral	D			
" Posters		A		

Materials Track

Symposium	W	Th	F	Sa
Design, Synthesis, and Characterization of Functional Polymeric Materials - Oral	D			
" Posters		A		
Polymer Blends and Composites - Oral			A	
" Posters		P		
Functional Inorganic Materials - Oral		D		
" Posters	P			
Sustainability and Recycling of Materials - Oral		D		
" Posters	P			

Organic/Medicinal Track

Symposium	W	Th	F	Sa
Illicit Fentanyl: A Perfect Storm in Science - Oral	D			
" Posters		A		
Cope Scholar Symposium: Enabling Approaches to Chemical Synthesis - Oral		D		
Advances in Catalysis for Organic Synthesis - Oral			D	

Biological Track

Symposium	W	Th	F	Sa
Biochemistry: Macromolecular Structure and Function - Oral		D		
" Posters	P			
Computer Simulations of Biochemical Processes: From Quantum to Classical and Back Again - Oral	D			
" Posters		A		
Biotechnology Innovation and Partnerships			D	

Education Track

Symposium	W	Th	F	Sa
Community College Chemistry Education: Successes and Strategies - Oral			A	
Generative AI: A Game-Changer for the Future of Learning and Research - Oral			P	
Evidence Based Pedagogies/General Chemistry - Oral			P	
" Posters		P		
Panel: Community College Transitions				A
Panel: New Two-Year College Guidelines				A

Special Event Lectures Track

Symposium	W	Th	F	Sa
James Seaba, ARPA E	P			
Karen Wooley, Texas A&M U	P			
Jacob Rosecrants, OK House of Rep.	P			
Bill Carroll, Ret.(ACS Past President)		P		
Angela Gronenbron, U Pittsburgh		P		
Kayunta Johnson-Winters		P		

Special Symposia Track

Symposium	W	Th	F	Sa
Diversity in Chemistry and STEM - Oral	D			
" Posters		A		
Best Practices for Successful Small Chemical Businesses - Oral		A		
Lessons and Inspiration from the History of Chemistry - Oral	A			
Innovative Ways to Convey the Value of Chemistry to the Public - Oral	P			

General Track

Symposium	W	Th	F	Sa
Analytical - Oral		D		
" Posters	P			
Biochemistry - Oral		P	A	
" Posters		A		
Inorganic - Oral	D	A		
" Posters		P		
Materials/Polymers - Oral			A	
" Posters		P		
Organic - Oral		P	D	
" Posters		P		
Physical - Oral	D	P		
" Posters		A		
Undergraduate - Oral			P	
" Posters			A	

Other Events

Some limited admission events may be full. Times and rooms might change. Check the on-line program for the most updated schedule.

Tuesday, November 14, 2023

Diversity Reception at the First Americans Museum, 6-9 PM

A reception at the First Americans Museum (FAM) will offer some inspirational stories of cultural diversity. In one place, visitors experience the collective histories of 39 distinctive First American Nations in Oklahoma today. ONE PLACE, MANY NATIONS. This reception is in conjunction with the Diversity in Chemistry and STEM at SWRM2023. The reception includes heavy hors d'oeuvres (roasted vegetables, turkey and wild rice meatballs, bison and green chile queso fundido), a cash bar, and admission to the Museum exhibits. Doors open at 6:00 pm, reception 6:30-8:00 with museum access and a guest speaker (TBA). FAM is 4 mi from the Omni Hotel. Participants are responsible for transportation to and from the venue.

Wednesday, November 15, 2023

Welcome Reception, 5:30-6:30 PM, Must be 21 years old to receive (1) free drink ticket.

Beer Tasting Seminar: Sensory Analysis and Beer-Tasting Lexicon, 8-9 PM

Join us for a sensory and lexicon-development session featuring local Oklahoma beers. Experience the different flavor compounds with a guided tasting led by Quality Control specialist Shawn Savuto of COOP Ale Works. Must be 21 years or older. The event will be held at one of the many OKC microbreweries, The Big Friendly (1737 Spoke St. Oklahoma City, OK 73108), 2.5 mi from the Omni Hotel. Participants are responsible for transportation to and from the venue. Food is available before the event at Taco Nation (open until 8 pm) next to The Big Friendly. The tap room will be open until 10 pm for continuing the discussion and sampling additional brews.

Thursday, November 16, 2023

Senior Chem Lecture and Breakfast, Oklahoma Station 8, 7-9 AM

Résumé Development: Marketing Your Brand for an Industrial Chemistry Position, Oklahoma Station 8, 9-11 AM

Provides an overview of the content of a robust résumé for an industrial chemistry position. Participants will also determine best practices in terms of résumé content and formatting through analysis of résumé exemplars. This workshop will also elaborate on the components of résumé portfolio, including cover letter and research summaries.

Women Chemists Committee Lecture and Lunch, Oklahoma Station 8, 12-1 PM

Grant Writing Workshop, Oklahoma Station 8, Thursday, Nov. 16, 2:30-4:30 PM

Ever wonder how you can improve the chances of your proposal being successful? What does the review panel really look for in a competitive proposal? This workshop will cover setting up the framework for a good proposal, common flaws in proposal writing, insights into the panel review process, and resubmission (if needed) best practices.

ACS Board Reception, South Prefunction, 5:30-6:30 PM (Check on-site program for times)

Symposium and Awards Banquet, Oklahoma Station 8, 6:30-8:30 PM (Check on-site program for times)

Friday, November 17, 2023

Active Learning Workshop, Oklahoma Station 8, 8:30-11 AM

Active learning/Higher engagement (AL/HE) teaching pedagogies are commonly discussed in chemistry education reform. There are many reasons - supported by published evidence - for why chemistry faculty should make AL/HE a prominent investment in their teaching portfolio. But what is oftentimes missing in the discussion is how to actually do/carry out AL/HE in the classroom. This workshop focuses on 'how to do' AL/HE and involves Think-Pair-Share, Jigsaw, and Just-in-Time Teaching strategies the workshop presenter uses in both GChem 1 and OChem 1. No theory. Just doing. Just applying.

Oklahoma Chemist of the Year, Lecture and Lunch, Oklahoma Station 8, 11:45-1:15 PM

Biotechnology Luncheon and Lecture, Oklahoma Station 7, 11:45-1:15 PM

Acing the Interview: Making the Most of Your Interview - Outshining the Competition (ACS), Oklahoma Station 8, 2-4 PM

Offers strategies and techniques to develop an extremely effective interview. Participants will also learn how to anticipate questions, develop thoughtful, robust responses, and handle difficult questions. The course will not only provide critical practice interview scenarios but will also help participants leave a lasting impression with hiring staff to secure the position well-aligned to their strengths and values.

Saturday, November 18, 2023

Presidential Workshop: Trust in Science, 8 AM-12 PM

This workshop is tailored for ACS members to use elements of humor to listen to and respond in conversations to other people's concerns, thoughts, and issues about a topic in science. Learn how ACS members can become trusted voices for science and scientists. Gain tools to equip members to advocate for this trust with all people - both those trained in science and those who are not. As chemists we know that despite the best efforts of all STEM professionals, even the greatest of scientific innovations and potential solutions cannot achieve their higher purpose if society does not trust and believe in the science and in the scientists telling the story.

Community College Transitions Panel, Route 66, 8:30-10 AM

New Two-Year College Guidelines Panel, Route 66, 10-11 AM

Community College Faculty Lunch with Panelists, Route 66, 11:30 AM -12:30 PM

Breaks

Wednesday Morning 9:30-10:30 AM, Prefunction

Wednesday Afternoon 2:15-3:30 PM, Expo

Thursday Morning 9:30-10:30 AM, Expo

Thursday Afternoon 2:15-3:30 PM, Expo

Friday Morning 9:30-10:45 AM, Expo

Friday Afternoon 2:15-3:30 PM, Prefunction

Saturday Morning 10:00-11:00 AM, Prefunction

Meeting Information

Hotel Venue

All sessions will be held in the OMNI Hotel, mostly on the second floor.

Poster Presentations

Poster Boards will be set up for use front and back. They should have a number on them corresponding to the paper number (1 to about 800). Each board should fit four 4 ft x 4 ft spaces (two on either side). Most posters are typically 3 ft x 4 ft. Diagrams and text should be readable from 3 to 4 ft back.

Poster Sessions will be held in the Mornings, 9-11 AM (Th, Fri) and afternoons 2-4 PM (Wed, Th, Fri). We understand that poster presenters not only wish to present their posters but also see other posters. To allow this freedom, we have the following guidelines.

Presenters with even numbers should be at their posters for the first hour of the poster sessions, and presenters with odd number presentations should be present during the last hour. During the other hour, you can visit the other posters and also spend some of the time at your own poster, as you see fit.

Posters can be set up 10 minutes before the session and taken down after the finish time. Push-pins will be provided.


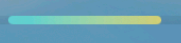

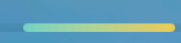








Oral Presentations

The current plan is for there to be a computer in each lecture room and presenters can show their presentation either by i) copying their presentation to the host computer and then displaying or ii) hooking up to their own computer (subject to Presiding Officer's permission). The pro-move is to bring both a pdf and presentation software (e.g., Powerpoint) on a jump drive. Your computer will require an HDMI output to the projection system. Even if you hope to use your own computer, bring a backup jump-drive presentation. Please try to introduce yourself to the Presiding Officer prior to the start of the session or during the break. A microphone and laser pointer will be available at the podium. Please leave 3-5 minutes of your allocated time for questions and allow transitions to the next presentation during this time.

Parking

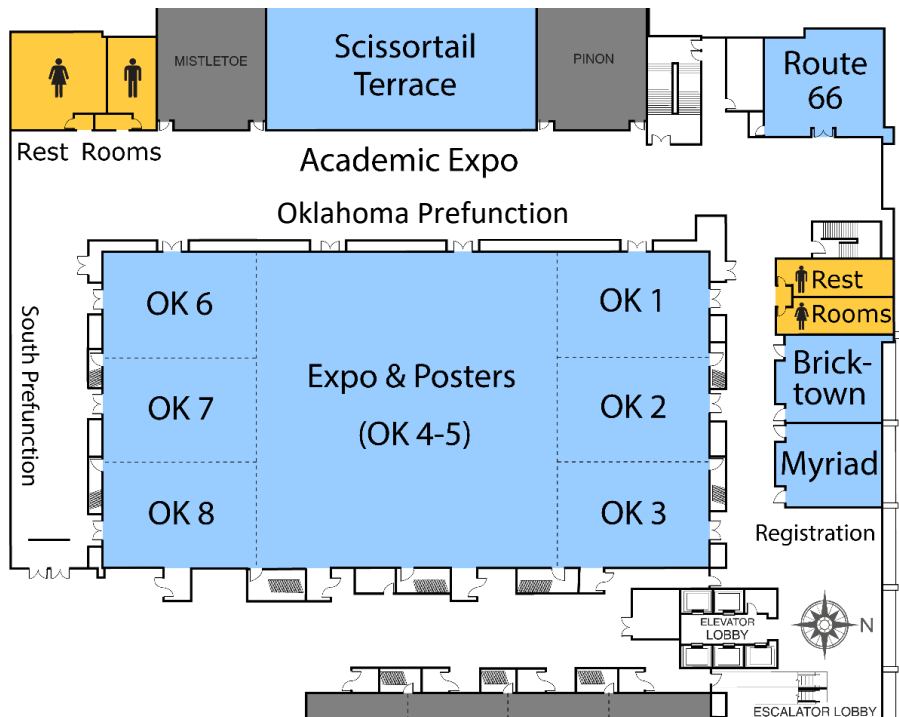
Lower cost parking is available at the parking lot just south of the Convention Center, Robinson Street between SW 6th and 7th. Caution: There is an OKC Thunder basketball game on Tuesday evening. Parking could be more complicated and perhaps more expensive then.

OKC Weather (or not)

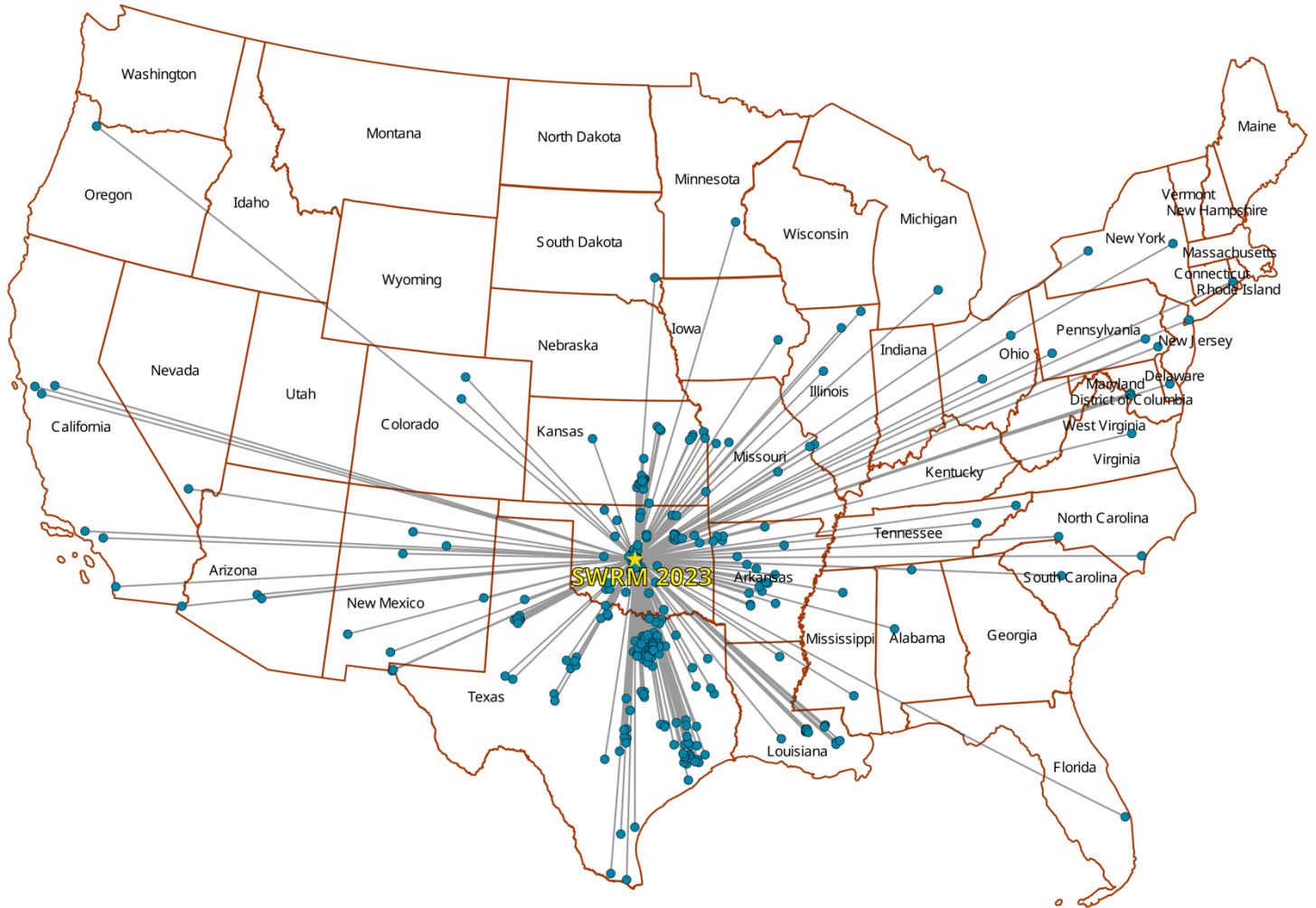
Tue		45°		67°
Wed		47°		69°
Thu		50°		68°
Fri		54°		68°
Sat		45°		67°
Sun		54°		63°



Omni Hotel Locations for SWRM 2023 Activities (2nd Floor, Omni)



SWRM Participation from USA



**Congrats to the organizers for an
awesome SWRM '23!**

Join us in **WACO** for **SWRM '24**



American Chemical Society

W ★ A ★ C ★ O

October 20-23, 2024



ACS SWRM 2023 Program Schedule

November 15-19, 2023

Oklahoma City, OK

F.D. Blum, *Program Committee Chair*

E. Schnitzler, *Program Committee Co-Chair*

Up-to-date November 13

CONTENTS

- 11 Wednesday morning
- 17 Wednesday afternoon
- 29 Thursday morning
- 39 Thursday afternoon
- 49 Friday morning
- 57 Friday afternoon

WEDNESDAY MORNING, November 15, 2023

Catalysis and Energy: Inextricable Links in the Chain of Progress

Omni Oklahoma City Hotel, Oklahoma Station 2

Cosponsored by CATL

S. Crossley, J.L. White, *Organizers, Presiding*

- 8:00** **1** Finding the needle in the haystack: Material discovery and design for electrocatalytic processes. **K. Gunasooriya**
- 8:20** **2** Leveraging non-covalent interactions for catalysis of electrochemical CO₂ reduction reaction. **A. Valles**, R. Hernandez Sanchez, V. Espinoza Castro
- 8:40** **3** Selective conversion of CO₂ to ethane through direct methanol coupling on two-dimensional MNene catalyst. **A. Djire**, B. Ngozichukwu, C. Ho Lee, D. Johnson, J. Kasten, J. Sang-Il Kwon
- 9:00** **4** Mechanistic studies of roles of extra-framework species in MFI zeolite on catalytic cracking of propane. **J.P. Crouch**, B. Wang
- 9:20** **5** Mechanistic details of pentanoic acid conversion over promoted molybdenum oxide. **L.A. Gomez**, C. Bavluka, T.E. Zhang, S. Crossley
- 9:40** **6** Radio frequency heating of catalyst systems. **A. Rout**, S.D. Lambert, D. Sengupta, M. Barteau, B. Wilhite, M. Green
- 10:00** Break.

- 10:20** 7 Effect of Brønsted acid site's local environment on zeolites' catalytic activities during acylation of 2-methylfuran with acetic acid. **I. Alalq**, V.T. Nguyen, L.A. Gomez, A. Zornes, J.L. White, B. Wang, S. Crossley
- 10:40** 8 Uncovering shifting catalytic phases in copper-based nanostructures during reverse water gas shift reactions. R. Addanki Tirumala, S. Ramakrishnan, **M. Khan**, M. Andiappan
- 11:00** 9 Catalytic conversion of natural gas and biomass to CO₂-free H₂ and carbon nanotubes over Ni-Mo-MgO catalyst. **P. Nguyen Thi**, L.A. Gomez, C. Bavlnka, I. Alalq, **S. Crossley**, D.E. Resasco
- 11:20** 10 Photocatalytic C-C coupling of terminal alkynes using hybrid Cu₂O-Pd nanostructures under ambient conditions. **R. Addanki Tirumala**, M. Andiappan
- 11:40** 11 Green process for producing carbon nanomaterials in rotary tube reactors. **R.A. Prada Silvy**

Computer Simulations of Biochemical Processes: From Quantum to Classical and Back Again 1

Omni Oklahoma City Hotel, Myriad

Cosponsored by PHYS

M. McCullagh, *Organizer*

G.A. Cisneros, *Organizer, Presiding*

H. Torabifard, *Presiding*

- 8:00** 12 Molecular simulations at the dawn of exascale computers: The age of agent-based computations. **A. Singharoy**
- 8:20** 13 What, how, and why of measuring conformational ensembles of biomolecules for molecular simulations. **M. McCullagh**
- 8:40** 14 A computational journey into long time-scale events: Nucleation and beyond. **B. Chen**
- 9:00** 15 Guiding proteins through conformational landscapes using anharmonic low-frequency vibrations. M.A. Sauer, S. Mondal, **M. Heyden**
- 9:20** 16 Ion selectivity and transport in novel microbial fluoride exporters. **H. Torabifard**
- 9:40** Break.
- 10:00** 17 Simulated pressure changes in LaCl suggest a link between hydration and functional conformational changes. N. Kariyawasam, **E.A. Ploetz**, L. Swint-Kruse, P.E. Smith
- 10:20** 18 Computational characterization of human orphan protein TMEM205. **F. Montalvillo**, H. Torabifard, G. Meloni
- 10:40** 19 Simulation studies of the self-assembly of sequence-defined singly and triply charged polypeptoids in aqueous solution. **R. Kumar**
- 11:00** 20 Structural insights into YAP/TAZ-TEAD interaction and its regulation by small molecules. **K. Mills**, J. Misra, H. Torabifard
- 11:20** 21 Multiscale simulations reveal the coupling between photochemistry and protein-ligand interactions in photopharmacology. **R. Liang**, A. Bakhtiari

Design, Synthesis, and Characterization of Functional Polymeric Materials

Omni Oklahoma City Hotel, Oklahoma Station 6

Cosponsored by POLY

C.E. Callmann, E. Pentzer, *Organizers, Presiding*

- 8:00 22** The future of polymer materials as the world progresses along the energy transition – dynamically-reconfigurable systems to unconventional sourcing of feedstocks: A story of pivots to overcome adversities while pursuing ambitions. **K.L. Wooley**
- 8:30 23** Synthesis and applications of chelating polymers. **P.R. Calvo**
- 8:50 24** Highly flexible dielectric films from solution processable covalent organic frameworks. **M.C. Senarathna**, H. Li, Y. Liu, R. Smaldone
- 9:08 25** Developing a novel, biomimetic, poly(δ -valerolactone)-based wound dressing. **C.K. Flynn**, S.K. Hamilton
- 9:26 26** Amine functionalized magnetic graphene oxide nanocomposite for rapid adsorptive removal of PFAS. S. Mahpishanian, **R. Foudazi**
- 9:51** Break.
- 10:11 27** Harnessing the reactivity of 2,3-pyridynes for the precise synthesis of main-chain cationic polymers with antibacterial properties. **Q. Michaudel**
- 10:36 28** Bismuth functionalized hydroxamic acid polymers as antimicrobial coatings. **S. Nawaz**
- 10:56 29** Efficient antifouling membranes for biopharmaceutical applications. **S. Tabatabaei**, R. Foudazi
- 11:14 30** On-demand drug delivery via photothermal modulation of dynamic covalent poly(ethylene glycol)/PEDOT composite hydrogels. K. Thapa, T. FitzSimons, M. Otakpor, M. Siller, A. Crowell, J. Zepeda, E. Torres, L. Roe, J. Arts, A. Rosales, **T. Betancourt**
- 11:34 31** Macromolecular post-synthetic electrochemical modification. **A.M. Evans**

Diversity in Chemistry and STEM

Omni Oklahoma City Hotel, Oklahoma Station 7

M.F. Borunda, *Organizer*K.L. Johnson-Winters, *Organizer, Presiding*

- 8:00 32** One science journey. **R. Snelling**
- 8:25 33** Aerospace engineering and applied mathematics summer academy for middle school girls. C. Rhodes, **E.A. Nalley**, L. Hale
- 8:50 34** A path less traveled - my untraditional journey in chemistry. **A. Hunter**
- 9:20 35** An account of my journey and my kinetic studies on F₄₂₀H₂:NADP⁺ oxidoreductase. **J. Howard**
- 9:45** Break.
- 10:05 36** Supporting diverse undergraduate students in STEM: Administrative and faculty perspective. **C. Valdez**
- 10:30 37** β -FeOOH nanoneedles as a precursor for the synthesis of Fe₃O₄ and FeS₂ nanoparticles. **Y. Vasquez**

- 10:55 38** Beyond large enrollments: Cultivating Latine student success in introductory chemistry through servingness-centered evidence-based pedagogies. **P. Vincent-Ruz**
- 11:20 39** Advancing diversity, equity, and inclusion in chemistry and STEM through 2D MXenes in renewable energy storage and conversion. D. Johnson, **A. Djire**

Illicit Fentanyl: A Perfect Storm in Science

Omni Oklahoma City Hotel, Oklahoma Station 3

D.J. Nelson, A.M. Timmons, *Organizers, Presiding*

- 8:00** Introductory remarks.
- 8:10 40** Illicit fentanyl: A perfect storm in science. **D.J. Nelson**
- 8:35 41** Fentanyl exposure: Facts vs. hysteria. **A.M. Timmons**
- 9:00 42** SHIFT: A UT Austin initiative to shift the conversation about substance misuse on campus in the fentanyl era. **B.L. Iverson**
- 9:25 716** The brain science of addiction and fentanyl FATE (Fighting Addiction Through Education, fate.org). **R. Whitten**
- 9:50** Break.
- 10:10 44** Fentanyl: The state of San Diego. **R.J. Harkins**
- 10:35 45** A discussion on the illicit fentanyl epidemic. D.J. Nelson, **C.C. Collier**, J. Macias, C. Gormley
- 11:00 46** Godfather of fentanyl. **D.J. Nelson**

Inorganic: Late Transition Metal Reactivity and Catalysis

Omni Oklahoma City Hotel, Route 66

R. Latifi, L. Tahsini, *Organizers*

M.B. Chambers, K.N. Green, *Presiding*

- 8:00 47** Mechanistic insights into copper-catalyzed oxidative decarboxylative coupling reactions. **J.M. Hoover**
- 8:20 48** Design principles of pincer-type Cu(I)-NHC complexes for bond activation and catalysis. **L. Tahsini**, R. Latifi, J. Raincrow, J. Minnick
- 8:40 49** Copper(I)-pincer bis-NHC catalyzed tandem carboxylation-esterification of terminal alkynes. **N. Back**, L. Tahsini
- 9:00 50** Synthesis and characterization of the para and meta substituted pyridine-based copper-bis(n-heterocyclic carbene) complexes and catalytic application in C-N and C-C cross coupling reactions. **J. Raincrow**
- 9:20** Break.
- 9:40 51** Macrocyclic molecule protects the lens from oxidative damage through multiple antioxidant pathways. **K.N. Green**
- 10:00 52** Rings of power: Effects of a secondary pyridine ring substitution on electronics and SOD activity of pyridinophanes. **K.J. Smith**, T. Schwartz, D.M. Freire, C. Bowers, K.N. Green

- 10:20 53** Direct photochemical C–H activation and C–C bond formation mediated by group (VI) dioxos. **M.B. Chambers**, S. Fosshat, S.M. Siddhiaratchi, C. Baumberger, V.Z. Valley
- 10:40 54** Speciation of a vanadium(V) catalyst for oxidative alcohol dehydrogenation studied with ¹⁹F and ⁵¹V NMR spectroscopies. J. Cerritelli, D. Fraser, C. Sabanos, S. Moore, **L.H. Doerrer**
- 11:00 55** Slurry of transition metal chalcogenides for multifaceted electrochemical applications: Energy conversion, storage, sensing and catalysis. **M. Nath**, H. Singh, I. Abdullahi, J. Masud, W.P. Liyanage
- 11:20 56** Placing gold on a π^+ -surface: Ligand design and impact on reactivity. **W. Liu**, F.P. Gabbai
- 11:40 57** Molecular electrocatalysts and their effect on CO₂ electrolyzers and redox flow batteries. **N. Mitchell**, N. Elgrishi

Lessons and Inspiration from the History of Chemistry

Omni Oklahoma City Hotel, Oklahoma Station 8

Cosponsored by HIST

C. Hahn, N.V. Tsarevsky, *Organizers, Presiding*

- 8:00** Introductory remarks.
- 8:05 58** Crafting the language of chemistry: Science, imagination, and art in collaboration. **N.V. Tsarevsky**
- 8:35 59** Bringing significant scientific discoveries to life: Executing a travel class that connects the history of science and chemistry with cultural events. **S.K. Hamilton**, S.E. Hubbard
- 9:05 60** Nuclear forensic analysis of Manhattan Project plutonium. **C.M. Folden**
- 9:35 61** Potassium nitrate, ammonium chloride and camphor: Together they changed the world immeasurably for the better – using some ethanol and water. **K.H. Pannell**
- 10:05 62** Franz Hein and the fascinating story of his "polyphenylchromium compounds". **C. Hahn**
- 10:30 63** Who was Wilhelm Dittmar? **C. Hahn**
- 11:00 64** Faraday's laws of electrolysis. **P. Kesavan**
- 11:30 65** Ergot alkaloids: A brief history. **L. Garcia**, N.V. Tsarevsky

Physical 1

Omni Oklahoma City Hotel, Bricktown

Y. Shao, *Organizer*

E. Schnitzler, *Organizer, Presiding*

K. Gunasooriya, *Presiding*

- 8:00 66** Chemistry below the barrier. **D.J. Bellert**
- 8:20 67** Atmospheric lifetime of primary brown carbon can be increased by ultraviolet irradiation. **H. Al-Mashala**, K.L. Betz, C. Calvert, J. Barton, E. Bruce, E. Schnitzler
- 8:40 68** Reaction of glyoxal and ammonium as a potential contributor to protein-like fluorescence in atmospheric aerosols. **A.W. Harrison**

- 9:00 69 Atmospheric aging of nanoplastics leading to hygroscopic partially-engulfed particles. **K.L. Betz**, H. Al-Mashala, E. Schnitzler
- 9:20 Break.
- 9:40 70 Electric field-induced second energy minimum of carbon monoxide. **D. Lai**, D. Matthews
- 10:00 71 PASSer: Prediction of protein allosteric sites through web service. **P. Tao**, H. Tian, S. Xiao
- 10:20 72 Effect of SARS-CoV-2 proteins on α -synuclein aggregation. **A.D. Chesney**, U. Hansmann
- 10:40 73 Rheological model fitting of nanoemulsions using the RhiNN algorithm: A study on large-amplitude oscillatory shear data. **B. Valipourgoodarzi**, R. Foudazi
- 11:00 74 Transfer machine learning of excited state energy corrections and reinforcement learning of tensor network contraction order. **I. Satyarth**, D. Matthews
- 11:20 75 Interaction of nisin with lipid molecules. **R. Sheridan**, U. Hansmann

Hydrocarbons: Exploration, Development, Refining and Processing

Omni Oklahoma City Hotel, Oklahoma Station 1

P.K. Bikkina, D. Papavassiliou, J. Weston, *Organizers, Presiding*

- 8:20 Introductory remarks. **D. Papavassiliou**.
- 8:25 76 Field applications of compact separators for multiphase production systems. **R.S. Mohan**
- 8:45 77 Review of downward liquid-gas flow characteristics in vertical pipes. **O. Osuagwu**, H. Karami
- 9:05 78 Liquid management in gas wells: Investigating the effects of tubular restrictions. **C.A. Mateus Rubiano**, M. Alsanea, H. Karami
- 9:25 79 Establishing a protocol for the study of the effectiveness of enhanced oil recovery techniques. S. Mtetwa, T.B. Berte, **M. Fahes**
- 9:45 80 Determination and comparison of oil swelling factors in the presence and absence of water for applications in CO₂ EOR and storage. **S. Pradhan**, P.K. Bikkina
- 10:05 Introductory remarks. **P.K. Bikkina**.
- 10:10 Break.
- 10:30 Introductory remarks. **W. Javen**.
- 10:35 81 Insights into rock-gas interactions under reservoir conditions: A case study from the late Mississippian Caney Shale, southern Oklahoma, USA. **F. Xiong**, G. Rother, G.A. Awejori, L. Bethel Dje, M. Radonjic
- 10:55 82 Cushion gas effects on clay-hydrogen-brine wettability at conditions relevant to underground gas storage. A. Ali, D. Cole, **A. Striolo**
- 11:15 83 Kinetics of high-yield carbon nanotube synthesis on lamellar clays. **C. Bavlnka**, M. Rhue, S. Crossley, B.P. Grady
- 11:35 84 Empirical relationships among density, viscosity, and total acid number (TAN) of crude oil. **P. Sapale**, S. Pradhan, P.K. Bikkina

WEDNESDAY AFTERNOON, November 15, 2023

Catalysis and Energy: Inextricable Links in the Chain of Progress

Omni Oklahoma City Hotel, Oklahoma Station 2

Cosponsored by CATL

S. Crossley, J.L. White, *Organizers, Presiding*

- 1:00 85** Polyolefin catalysis – industrial perspectives. **M.D. Refvik**, M. McDaniel, Q. Yang
- 1:20 86** Ethylene polymerization by the Phillips Cr/silica catalyst. **M. McDaniel**
- 1:40 87** Metallocene catalysts in polyethylene synthesis. **Q. Yang**, M.P. McDaniel, M.D. Refvik
- 2:00 88** Understanding how polyolefin properties affect reactivity and diffusivity over solid acid catalysts. **A. Jerdy**, M. Gonzalez Borja, M. Monwar, L. Lobban, S. Crossley
- 2:20** Break.
- 2:40 89** Tailoring zeolite catalysts for sustainable energy. **H. Cho**
- 3:00 90** Exploring new pathways for coupling CO₂ and C₂H₄ to form acrylic acid on atomically dispersed M-O-M di-atomic sites in MFI zeolites. **Z. Masood**, B. Wang
- 3:20 91** Impact of low-temperature water exposure and removal on zeolite HY. **A. Zornes**, O. Das, N. Abdul Rahman, S. Crossley, D.E. Resasco, J.L. White
- 3:40 92** The promotional effect of water on the hydrogenation of cyclohexene over nickel boride. **T. Salas**, D.E. Resasco
- 4:00 93** Investigating the interplay of hydrogen transfer, protolytic cracking, and dehydrogenation reactions over faujasite zeolites by using isooctane conversion as a probe. **N. Abdul Rahman**, N.F. de Paula, P. Nguyen, R. Bababrik, W.E. Alvarez, M.J. Wulfers, S. Crossley, D.E. Resasco
- 4:20 94** Intermediate transfer rates and solid-state ion exchange are key factors determining the bifunctionality of a tandem CO₂ hydrogenation catalyst. **F. Mahnaz**, J. Mangalindan, M. Shetty

Computer Simulations of Biochemical Processes:

From Quantum to Classical and Back Again 2

Omni Oklahoma City Hotel, Myriad

Cosponsored by PHYS

G.A. Cisneros, *Organizer*

M. McCullagh, *Organizer, Presiding*

D. Girodat, *Presiding*

- 1:00 95** The role of polarization in the conformation distribution of hydrated peptides: Dipole cooperativity and dielectric frustration. **F. Wang**, Y. Yuan
- 1:20 96** Design of bio-based ionic liquids using multipolar-polarizable force field. **S. Heidari**
- 1:40 97** Can different solvents change an enzymatic reaction mechanism? The case of HRP. **G.A. Cisneros**
- 2:00 98** Computational investigation of unnatural base pairs (UBPs) in DNA in solvent and in ternary complex in a DNA polymerase. **T. Debnath**, G.A. Cisneros

- 2:20 99** Accurate mRNA decoding is reinforced by aminoacyl-tRNA alignment relative to catalytic centers of the ribosome. **D. Girodat**, H. Wieden, S. Blanchard, K.Y. Sanbonmatsu
- 2:40** Break.
- 3:00 100** Per- and polyfluorakyl substances (PFAS): A (bio)molecular-level approach towards impact and mitigation strategies. S. Bali, N. Almeida, N. Loganathan, **A.K. Wilson**
- 3:20 101** Motif-VI loop acts as a valve for nucleotide in the WNV NS3 helicase. **P. Roy**, M. McCullagh
- 3:40 102** QM/MM and molecular dynamics simulations to decipher the reaction mechanism of the Cas9 HNH domain. **V.M. Jayasinghe Arachchige**, Y. Maghsoud, P. Kumari, G.A. Cisneros, J. Liu
- 4:00 103** Combining machine learning potential and molecular mechanics for free energy simulations of enzymatic reactions. **X. Pan**, Y. Shao
- 4:20 104** A tale of two sides of enzymes: Stories of catalytic mechanisms and dynamics told through machine learning. **P. Tao**

Diversity in Chemistry and STEM

Omni Oklahoma City Hotel, Oklahoma Station 7

K.L. Johnson-Winters, *Organizer*

M.F. Borunda, *Organizer, Presiding*

- 1:00 105** Anti-discrimination, equity, and inclusivity lead to diversity. **A. Augustus-Wallace**
- 1:25 106** NanoExplorers: A high school summer science academy. **E.A. Nalley**, C. Rhodes
- 1:50 107** A colorful journey from academia to industry – my reflections on a career path in the chemical industry with Native American ancestry. **C. Brown**
- 2:15 108** Threshold displacement energies in organic and inorganic halide perovskites from ab initio molecular dynamics. **R.B. Martinez Duque**, M.F. Borunda, I. Sellers, A. Kirmani
- 2:40 109** Polymeric nanoparticles as photothermal agents for cancer therapy and on-demand drug delivery. **T. Betancourt**
- 3:05** Break.
- 3:25 110** Engaging general chemistry students through DEI projects and current STEM social issues. **C. Fulton**
- 3:50 111** Kinetic and biophysical characterization of F₄₂₀ cofactor-dependent glucose-6-phosphate dehydrogenase (FGD) variants from *Mycobacterium tuberculosis*. **L. Davis**, M. Oyugi, A. Aziz, K.L. Johnson-Winters
- 4:15 112** From kitchen chemist to a global solution – how vision, experience and education lead (leadership, education, and development) to finding purpose. **S. Perry**

Illicit Fentanyl: A Perfect Storm in Science

Omni Oklahoma City Hotel, Oklahoma Station 3

D.J. Nelson, A.M. Timmons, *Organizers, Presiding*

- 1:00 113** Fentanyl analogs: Developing new analytical methods for detection. **A.M. Timmons**

- 1:25 114 Addiction and the rise of fentanyl – a driving force in the criminal justice system. **J. Stoner**
- 1:50 115 Assessing the extraction efficiency of fentanyl and fentanyl analogs from household surfaces. **A. Ciesielski**
- 2:15 116 Fentanyl – it's a big deal. **T.C. Kupiec**
- 2:40 Break.
- 3:00 117 Fatal fentanyl: Overdose deaths at the Oklahoma Office of the Chief Medical Examiner. **K. Cliburn**, K.A. Brogden, C. Yacovazzi, J. Kemp
- 3:25 118 Overcoming challenges associated with fentanyl analysis in analytical laboratories: From sample preparation to LC-MS/MS analysis. **S. Olive**
- 3:50 119 Oklahoma's fentanyl epidemic from a law enforcement perspective. **M. Woodward**
- 4:45 120 Review of current activities in the Oklahoma House of Representatives. **J. Rosecrants**, D.J. Nelson
- 4:40 Concluding remarks.

Innovative Ways to Convey the Value of Chemistry to the Public

Omni Oklahoma City Hotel, Oklahoma Station 8

S.R. Goode, *Organizer*

H. Cheng, *Organizer, Presiding*

- 1:00 Introductory remarks.
- 1:05 Remarks by immediate past President. **A. Wilson.**
- 1:20 121 Strategically communicating chemistry. **L. Houston**
- 1:45 122 Utility of the performing arts as educational tools and in communicating the value of chemistry to the public. **N.V. Tsarevsky**
- 2:10 123 Chemists should write like journalists and talk like cavemen. **R.C. Fortenberry**
- 2:35 124 Cowboy chemistry and small-town science: Using podcasting and local libraries to increase chemistry literacy, relatability, and accessibility. **D. Eralie**
- 3:00 Break.
- 3:15 125 OCAST: Igniting Oklahoma's tech and innovation surge. **J. McGrail**
- 3:40 126 Challenges and opportunities in science education in post-COVID era and corporate involvement. **M. Monwar**
- 4:05 128 ACS resources for communicating the value of science to the public. S.R. Goode, **H. Cheng**

Inorganic: Main Group Element Reactivity and Catalysis

Omni Oklahoma City Hotel, Route 66

R. Latifi, L. Tahsini, *Organizers*R. Comito, R.D. McCulla, *Presiding*

- 1:00 129** Visible light induced photodeoxygenation of polycyclic selenophene Se-oxides. **R.D. McCulla**
- 1:20 130** Applications of the fluorophilicity of germanium: Hydrodefluorination of acid fluorides and organofluorine compounds using organogermanes. **C.S. Weinert**, V. Fortney, A. Hayatifar
- 1:40 131** Formation of amide bonds using acid fluorides and germylamines: A versatile method for the generation of the peptide linkage. **V. Fortney**, T. Stancil, J. Murphy, C.S. Weinert
- 2:00 132** Acceleration of near-IR emission through efficient surface passivation in Cd₃P₂ quantum dots. **I. Fedin**
- 2:20** Break.
- 2:40 133** Bimetallic main-group catalysts for the synthesis of advanced biodegradable polymers. **R. Comito**, M. Tansky, J. Qian
- 3:00 134** Anion binding in solution through bidentate pnictogen and chalcogen host systems. **C. Bateman**, J. Qiu, A.F. Cozzolino
- 3:20 135** Synthesis and reactivity of base-supported organobismuth Lewis acids. **N.H. Hunter**, F.P. Gabbai
- 3:40 136** Analyzing fluoride binding by Group 15 Lewis acids: pnictogen bonding in the pentavalent state. **L. Maltz**, F.P. Gabbai
- 4:00 137** Sequestration of “forever chemicals” from water with a self-assembled metallo-cage. **M. Das Bairagya**, S. Ntipouna, N. Elgrishi
- 4:20 138** Chlorinated *o*-catecholostiboranes as Lewis acids. **F. Sit**

Physical 2

Omni Oklahoma City Hotel, Bricktown

E. Schnitzler, Y. Shao, *Organizers*D. Bellert, K. Onchoke, *Presiding*

- 1:00 139** Effect of sulfur hybridization on methanethiol adsorption geometry on unrelaxed Au(111). S. Bhattacharya, G. Speyer, D.K. Ferry, **L.A. Bumm**
- 1:20 140** Influence of wettability and step-down pressure on pressure-driven bubble nucleation in supersaturated gas-liquid systems. **S. Pradhan**, P.K. Bikkina
- 1:40 141** Physicochemical properties of per- and polyfluoroalkyl substances (PFAS) at the air-water interface. **M. Zhou**, R. Foudazi
- 2:00 142** Microfluidic-based evaluation of flow dynamics of ionic liquids (ILs) for enhanced geothermal systems. **C. Akhilome**, S. Pradhan, P.K. Bikkina
- 2:20 143** Temperature dependence of polar aggregation in ionic liquids: the example of 1-methyl-1-butyl-pyrrolidinium bis(trifluoromethylsulfonyl)imide. **R.A. Wheeler**, E.E. Dalbey, N.A. Mauro

- 2:40 Break.
- 3:00 144 Influence of surfactant molecular dynamics and intramolecular interactions on surface tension reduction. **T. Kobayashi**, K. Kotsi, T. Dong, I. Mcrobbie, A. Moriarty, P. Angeli, A. Striolo
- 3:20 145 Implementation of energy and gradient for the TD-DFT-approximate auxiliary function (aas) method. **Y. Wang**, C.M. Aikens
- 3:40 146 Localized tensor hypercontraction in quantum chemistry. **J. Thorpe**, D. Matthews
- 4:00 147 Implementing semiempirical methods for excited state processes. **C. Lander**, Z. Pei, X. Pan, Y. Zhang, Y. Shao
- 4:20 148 High-performance computation of electron repulsion integrals with SYCL. **D. Jiang**, C. Yin, A. Delgado, D. Matthews

Solar, Fuel, Wind and Future Energy

Omni Oklahoma City Hotel, Oklahoma Station 1

L. Ford, *Organizer*

J.L. Liu, J. Titah, *Presiding*

- 1:00 149 Remote renewable to liquids. **J. Seaba**
- 1:25 150 Design of solar-powered desalination systems for remote areas. **K. Alanazi**, M. Tarawneh, K. Hakami, A. Almasoudi, R. Mohan
- 1:45 151 Diglyme-based structural battery electrolytes produced by polymerization-induced phase separation for low-temperature applications. **S. Deshpande**, V. Vidyaprakash, S. Oka, C. Wang, K. Liu, M. Green, J.L. Lutkenhaus
- 2:05 152 A dye-sensitized photo-supercapacitor using commercial carbon-based materials as the intermediate electrode. **V. Bishop**, W. Wei
- 2:25 153 Enhanced performance of supercapacitors composed of flexible metal oxide electrodes with tunable structure. **J.L. Liu**, S. Bashir
- 2:45 Break.
- 3:05 154 Thermo-hydro-electrochemical effect. **Y. Zhang**, A. Sohn, A. Chakraborty, C. Yu
- 3:25 155 Ti₂N nitride MXene for green ammonia production: Mechanistic understanding through in-situ spectroelectrochemistry. **D. Johnson**, R. Yoo, A. Djire
- 3:45 157 Porous inorganic-organic framework polyhedral oligomeric silsesquioxanes (POSS) as hydrogen storage materials. **D. Hossain**
- 4:05 158 Exploring the role of homopolar dihydrogen bonding in stabilizing the solid-state structures of hydrogen storage materials: A computational approach. **J. Titah**

Design, Synthesis, and Characterization of Functional Polymeric Materials

Omni Oklahoma City Hotel, Oklahoma Station 6

Cosponsored by POLY

C.E. Callmann, E. Pentzer, *Organizers, Presiding*

- 1:20 159** Phase behavior of polymer-grafted nanoparticle blend films via thermal and solvent vapor annealing. **A. Karim**, A. Gul, K. Sharma, J. Transangpradit, M.R. Bockstaller, K. Matyjaszewski
- 1:50 160** Unveiling nanoscale domain formation and hierarchical self-assembly in polymer blends through infrared nanoimaging. **T.G. Habteyes**
- 2:08 161** Charge transfer in spatially defined organic radical polymers. **E.M. Fox**, T. Ma, M. Qi, C. Li, K. Sachinthani, K. Mohabty, D.P. Tabor, E. Pentzer, J.L. Lutkenhaus
- 2:26 162** Amide activation as a platform for diverse functional materials. **A. Teator**
- 2:51** Break.
- 3:11 163** Photoresin design for smart, functional 3D printing. **R. Smaldone**
- 3:36 164** Functionalized polymeric electrolyte used to improve electrochemical property and long-term stability of microbial fuel cells. S. Bashir, W. Houf, **J.L. Liu**
- 3:56 165** Morphological engineering of conjugated polymers for next-generation electrochromic devices. **R.M. Pankow**
- 4:16 166** Harnessing the power of natural products towards the synthesis of high-performance materials. **S.L. Kristufek**

Analytical Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

S. Gamagedara, *Organizer***2:00 - 4:00**

- 167** Competitive dissociation reactions of ternary complexes containing Ni(II), nitrilotriacetic acid and alternative metal binding peptides. **P. Asare**
- 168** Electroanalysis of pH and packaging effects on meat discoloration. **S. Ayabadda Devage**, S. Dias, S. Bhandari, A. Avery, R. Kumar, R. Ramanathan, S. Krishnan
- 169** Single molecule spectroscopy and super-resolution microscopy imaging with ultrahigh-throughput. **J.E. Batey**, G. Kim, M. Yang, D. Heffer, E. Pott, H. Giang, B. Dong
- 170** Electrochemical study on the discoloration of normal beef sarcoplasm pH dependence and storage effect. **S. Bhandari**, S. Dias, S. Ayabadda Devage, R. Kumar, R. Ramanathan, S. Krishnan
- 171** Using high pressure liquid chromatography to evaluate evaporation of dimethyl trisulfide from aqueous solutions. **D. Brockhausen**, A. Newton, D.E. Thompson
- 172** Analysis of the surface interactions between polyethylene microplastics and sodium lauryl ether sulfate. **X. Webb**, G.A. Salazar
- 173** Thermochemical studies of Ni(II) ternary complexes of alternative metal binding peptides. **J. Morlaes**, L.A. Angel

- 174 Energy-resolved threshold collision-induced dissociation of zinc(II) ternary complexes of alternative metal binding peptides with nitrilotriacetic acid. **K. Senyah**
- 175 Point-of-need colorimetric sensor for insulin monitoring. **S. Samaraweera**, Z. Syed, S. Krishnan
- 176 Attaining true multicolor STORM images using phasor analysis. **E.D. Pott**, M. Yank, J. Batey, B. Dong
- 177 Mass spectrometry imaging of very long chain fatty acids in brain of spinocerebellar ataxia 34 rat model in negative polarity. **D. Chen**, Z. Zou, E.A. Adewunmi, R.S. Brush, A.J. Brown, M. Agbaga, Z. Yang
- 178 Extraction of soybean oil using green solvents and techniques. **C. Mcdowell**, **M. Oum**, S. Dharmarajan
- 179 Assessing ecofriendly Louisiana waste products in removal of pyrene and chrysene as models of oil spills. **F. Louka**, **J.H. Smith**, S.Y. Osman
- 180 Mercury amalgamation effect on three-dimensional orientation of mesoporous silica coated gold nanorods at the single particle level. **G. Kim**, B. Dong
- 181 Field-amplified sample injection coupled with electrokinetic supercharging for sensitive detection of herbicide residues by flow-gated capillary electrophoresis. **Y. Gong**, M. Gong
- 182 Efficacy evaluation of ion exchange and acid precipitation methods for depleting serum abundant proteins using bottom-up proteomics. **Z. Peng**, W. Shakya Sankalpani Gunasena, D. Bhusal, I. Yang, N. Ahsan, Z. Yang
- 183 Effect of multidrug resistance on drug-uptake in cancer cells and spheroids. **A. Singh**, Z. Peng, A. Huynh, A.W. Burgett, Z. Yang

Biochemistry: Macromolecular Structure and Function Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

Cosponsored by CARB

R. De Guzman, S. Mohanty, *Organizers*

2:00 - 4:00

- 184 Probing conformational changes that gate electron transfer in bifurcating FixABCX from *Azotobacter vinelandii*. **N. Mohamed Raseek**, F. Ghorbani, F. Mus, M. Tokmina-Lukaszewska, B. Bothner, J. Peters
- 185 Bridge helix modulation of Cas9 as an efficient protein engineering method to improve on-target DNA cleavage fidelity. **C. Ganguly**, **K. Long**, D. Wu, P.Z. Qin, R. Rajan
- 186 Characterization of an insect pheromone binding protein: Implications for environmentally friendly pest management. **P. Paudel**, O. Al Danoon, S. Ayyappan, S. Mohanty
- 187 Synthesis of novel tryprostatin B analogs containing chemoselective functionality using prenyltransferase CdpNPT. **L. Coleman**, D. Dimas, S. Singh
- 188 In-vitro glycosylation of two ectodomain of syndecan-1 using *n*-glycosyltransferase. **W. Than**, J. Bryce, G. Cook
- 189 Analysis of toxicity effects of different silica NPs morphologies on a human gut model. **M. Sheikh Yamin**

- 190 Utilizing membrane protein chaperone to prevent and disrupt alpha synuclein protein aggregation in Parkinson disease. **I. Makelaar**, F. Liang
- 191 Leveraging membrane protein chaperones to mitigate familial mutant amyloid beta aggregation: Prospective therapeutic approach for early-onset Alzheimer's disease. **A. Vann**, F. Liang
- 192 Isolation and characterization of a bacterial mutant strain deficient for the pyrimidine biosynthetic enzyme orotate phosphoribosyltransferase. **S. Bodampati**, B.S. Duran-Pena, T.P. West
- 193 Characterization of a bacterial mutant strain deficient for the pyrimidine biosynthetic enzyme orotidine 5'-monophosphate decarboxylase. **L.V. Gore**, B.S. Duran-Pena, T.P. West
- 194 Extraction and evaluation of gaillardin as an HDAC inhibitor in A375 and MDA-MB-231 cancer cell lines. **N. Pyenta**, **O. Uzumefune**, **J. Gribble**, P.S. Pyenta, H. Shin
- 195 Glycosylation of full-length human γ -sarcoglycan in nanodiscs. **J. Ewusi**
- 196 Focused look at the transmembrane domain of the glycoprotein gamma-sarcoglycan. **J. Bryce**, J. Ewusi, M. Harris, G. Cook
- 197 Expression, purification, and characterization of T-cell receptor alpha (TCR α) and transmembrane serine protease II (TMPRSS2). **T. Ogunleye**, G. Cook
- 198 CooB catalyzed the refolding of the CS1 pilus subunit CooA. **P. Loh**, J. Bann
- 199 Membrane protein chaperone modulates the kinetics and morphology of tau aggregation: A potential treatment for Alzheimer's disease. **K. Rodgers**, F. Liang
- 200 ^{19}F -NMR studies reveal dynamic behavior upon pore formation of the binding domain of the anthrax toxin protective antigen. **R. Karimi**, J. Bann
- 201 Characterization of F₄₂₀ dependent glucose-6-phosphate dehydrogenase from *Nocardioideae bacterium*. **M. Ahamed**
- 202 Structural determinants for metal preferences in acetone carboxylase. **T. Flusche**, K. Shisler, F. Mus, J. DuBois, J. Peters
- 203 Rational remodeling of FnCas12a active pocket to abrogate non-specific cleavage activities. **S. Rostami**, R. Van, M. Shelton, Y. Shao, R. Rajan
- 205 Journey to molecular visualization of Asian corn borer olfactory protein. **P. Combs**, S. Ayyappan, J. Russell, S. Mohanty
- 206 ^{19}F -NMR studies of a dominant-negative mutant of the anthrax toxin protective antigen. **S. Gonti**
- 207 Characterization of cardiomyopathic point mutations of the Ig3 domain in myopalladin. **J. Tran**, A. Michaelis, A. Arachchige, M. Beck
- 208 Tyrosine hydroxylase in dopaminergic neuron cells lead to increased oxidative stress and cell death by activation of acidosis. **M.M. Eldani**, **O.A. Adetuki**, K. Wimalasena
- 209 Role of palladin in actin dynamics revealed by quantitative TIRFM. **S. Ghimire**, T. Izard, W. Yessin, M. Beck
- 210 Alzheimer's disease treatments: Their mechanisms of action. **A. Rahman**, A. Pan
- 211 Investigations of G-triplex DNA formation by surface plasmon resonance. M. Myhre, W.M. David, **S.M. Kerwin**

- 212** Inhibition of amylin aggregation by heat shock cognate 70 molecular chaperones. **N. Saikia**, A. Chaari, F. Ding
- 718** Self-assembly of a fluorescent virus-like particle for imaging in tissues with high autofluorescence. **I. Trashi**, M.Z. Durbacz, O. Trashi, Y.H. Wijesundara, R.N. Ehrman, A.C. Chiev, C.B. Darwin, F.C. Herbert, J. Gadhvi, N.J. De Nisco, S.O. Nielsen, J.J. Gassensmith
- 719** Surface modified dendrimers for slow release of active ingredients. **O. Trashi**, N. Satish, I. Trashi, L. Hagge, Y. Wijesundara, J.J. Gassensmith

Functional Inorganic Materials Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

Cosponsored by COLL

Financially supported by J. Luminescence Materials Advances

J. Chan, B. Saparov, Y. Vasquez, *Organizers*

2:00 - 4:00

- 213** Fluoride-free synthesis of two-dimensional titanium carbide based MXene ($Ti_3C_2T_x$). **A. Ahouei**, W. Wei
- 214** Heteroanionic $LaBrVIO_4$ (VI = Mo, W): Excellence in both nonlinear optical properties and photoluminescent properties. **Z. Jiao**, J. Wang
- 215** Sequence dependent self-assembly of ssDNA oligonucleotides onto boron nitride nanotubes: Insights on the free energy landscape using molecular dynamics simulation. **N. Saikia**
- 216** Electrochemical sensing of cadmium ion via functionalized carbon dots prepared by bottom-up approach. **J. Mbese**
- 217** $Li_2MP_2S_6$: A family of 2D van der Waals layered materials and their physical properties. **S. Sundaramoorthy**, N. Gerasimchuk, K. Ghosh, A. Choudhury
- 218** Role of fluoro-bridged clusters in rare-earth metal-organic frameworks. **M. Abbas**, K.J. Balkus
- 219** Computational investigation of cooperativity in intermolecular iodophilic interactions of an oxidative-addition gold trimer black absorber. **J. Adebajo**, M. Custer, M.M. Ghimire, **M.A. Omary**
- 220** Exploring InSb quantum-well structures for geometric diodes. **S. Aravindan**, M. Santos
- 221** Understanding the effect of moderate concentration SDS on CO_2 hydrates growth in the presence of THF. **X. Cai**, J. Worley, A. Phan, M. Salvalaglio, C.A. Koh, A. Striolo
- 222** Diffusion controlled synthesis and growth of cesium lead bromide nanocrystals. **S. Chandra**, C. Mi, Y. Dong
- 223** Versatile metal nanoparticles can be easily, safely, and cost-effectively synthesized through a green chemical process using hydrophilic polypeptide-rich aqueous extracts from insects, arthropods, and microorganisms. **J.L. Cho**, **M. Ward**, H. Galmiche, W. Yang, L. Allain, S. Liu, P. Wang, M. Boulido, R.E. Evans
- 224** Impact of hard water on calcium carbonate-stabilized Pickering foams. **A. Copelin**, E. Lima Correia, S. Razavi
- 225** Computational design of novel 2D aXMene for prospective applications in electrochemistry. **U. De Alwis**, V. Choutipalli, K.L. Shuford

- 226 Hydrogen transport mechanisms through amorphous polyethylene matrices studied via molecular dynamics simulations. **C. Divine-Ayela**, F. Perez Valencia, A. Striolo
- 227 Surface effects on biexciton auger efficiency in single CsPbBr₃ quantum dots. **G.C. Gee**
- 228 Cluster seeded doping of perovskite quantum dots. **L. Hidayatova**
- 229 Chemical vapor deposition synthesis, characterization, and photoluminescence of β -gallium oxide nanostructures. **M. Jaekel**, L. Marder, T.M. Trad
- 230 Singlet oxygen involved in activation of peroxymonosulfate by recyclable Co_{0.5}Mn_{0.5}Fe₂O₄ for tetracycline degradation. **M. Ifires**, A. Barras, T. Hadjersi, R. Boukherroub, S. Szunerits
- 231 Light-triggered release of indocyanine green using polydopamine-coated gold nanocages. **E. Knight**, S. York, D. Okyere, J. Chen
- 232 Catalytic transformation of azide-modified gold nanoparticles via visible light activation for biomedical applications. **M. Naderi**, S. Sulthana, J.D. Weaver, Y. Vasquez
- 233 Comparative analysis of structural and physical properties of two distinct two-dimensional lead halides with intercalated Cu(II). **K. Parashar**, Z. Zhang, B. Saparov
- 234 Electronic structures and optical properties of new hybrid organic-inorganic metal halides [(CH₃)₃SO]M₂l₃ (M = Cu, Ag). **T. Pinky**, D. Popy, Z. Zhang, B. Saparov
- 235 Intermetallic single crystal growth optimization by DSC. **M. Plata**, A. Dominguez, J. Chan
- 236 Investigation of Sn-based chalcogenides as electrocatalysts for selective reduction of CO₂. **A. Rozhkova**, I. Abdullahi, M. Nath
- 237 Nanometer-scale optoelectronic characterization of 1, 4, 8, 11, 15, 18, 22, 25-octabutoxyphthalocyanine oriented ultra-thin single-crystals. **S. Raybould**, T.H. Joyee, V. Mapara, M. Furis, **L.A. Bumm**
- 238 Synthesis and characterization of zinc and manganese ferrite nanoparticles and their efficacy against Xanthomonas pathogens. **M. Sehlaoui**, L. Marder, T.M. Trad
- 239 Iron phosphide nanobundles for efficient electrochemical hydrogen evolution reaction (HER) in acidic and alkaline media. **S. Sharma**, N. Khatri, M. Adhikari, K. Kalkan, Y. Vasquez
- 240 Gold nanoparticle encapsulation in flower-like wrinkled mesoporous silica. **A. Siddiki**, V. Poruri, K.J. Balkus
- 241 Developing analytical algorithms for the rapid identification of atomically thin materials. **S. Sreeram**
- 242 Greenish white to orange-red: Anion modulated near unity photoluminescence in interconvertible hybrid copper halides and their multimodal luminescent anti-counterfeiting and WLED applications. **D. Popy**, B. Saparov
- 463 Polymorphism study of Ce₂MnGe₆. **M. Raines**

Hydrocarbons: Exploration, Development, Refining and Processing Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

P.K. Bikkina, *Organizer*

D. Papavassiliou, *Presiding*

2:00 - 4:00

243 Metal free reassociating preformed particle gels for high temperature oil well treatments. **Y. Eriyagama**, T.P. Schuman, B. Bai, K.H. Woelk

244 Molecular dynamics simulations reveal how corrosion inhibitor influences the performances of kinetics hydrate inhibitor. **T. Le**, A. Striolo

Sustainability and Recycling of Materials Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

H. Cheng, R. Vaidyanathan, *Organizers, Presiding*

2:00 - 4:00

245 Selective dehydration of poly(vinyl alcohol-co-ethylene) using Pd/MOO₃ as a catalyst. **S. Abdolbaghi**, S. Crossley

246 Surface modified TiO₂ nanoparticles for photocatalytic water treatment. **W. Wilber**, S. Ramasamy

247 Post-consumer poly(ethylene terephthalate) carpet and recycled mixed polyolefin resin composites. **A. Nayar**, A. Maheshwari, R. Azarfam, F.D. Blum, R. Vaidyanathan

250 Circular economy models for smartphones – a case of Taiwan. **S. Rikitu**

251 Applying circular economy strategies to find solutions for SDG 12s: E-waste management case studies. **S. Rikitu**

Wednesday Special Event Lectures

Special Event Lecture

Omni Oklahoma City Hotel, Oklahoma Station 1

F.D. Blum, L. Ford, *Organizers*

L. Ford, *Presiding*

4:45 - 5:30

252 GREENWELLS, Grid-free Renewable Energy Enabling New Ways to Economical Liquids and Long-term Storage. **J. Seaba**

Special Event Lecture

Omni Oklahoma City Hotel, Oklahoma Station 3

D. Nelson, *Organizer, Presiding*

4:45 - 5:30

120 Review of current activities in the Oklahoma House of Representatives. **J. Rosecrants**

Special Event Lecture

Omni Oklahoma City Hotel, Oklahoma Station 6

F.D. Blum, E. Pentzer, C. Callman, *Organizers*

E. Pentzer, C. Callman, *Presiding*

4:45 - 5:30

720 Sustainable plastics from sugar. **K. Wooley**

THURSDAY MORNING, November 16, 2023

Biochemistry: Macromolecular Structure and Function

Omni Oklahoma City Hotel, Myriad

S. Mohanty, *Organizer*R. De Guzman, *Organizer, Presiding*N. Saikia, *Presiding*

- 8:00** Introductory remarks.
- 8:05 253** Uncovering the conformational dynamics of the hepatitis C virus 3' X RNA. P. Sperstad, **E.D. Holmstrom**
- 8:30 254** Simultaneous inhibition of two neutrophil serine proteases by the *S. aureus* innate immune evasion protein EapH2. **O. Prakash**, N. Mishra, T. Herdendorf, B. Geisbrecht
- 8:55 255** Elucidating the molecular determinants governing the bias in [FeFe]- hydrogenases. **B. Jagilinki**, D. Mulder, E.C. Kisgeropoulos, P.W. King, J.W. Peters
- 9:15 256** Threshold collision-induced dissociation of Ni(II) and Zn(II) ternary complexes of alternative metal binding peptides with nitrilotriacetic acid. **L.A. Angel**, K.N. Senyah, P. Asare, J.D. Wilcox, J. Morales
- 9:35 257** *in vitro* glycosylation of membrane proteins involved in human disease. **G. Cook**
- 10:00** Break.
- 10:20 258** RuvC active site engineering to develop stringent Cas9 variants for safer genome applications. **R. Rajan**, S. Newsom, S. Rostami, P.Z. Qin, J. Liu, D. Wang
- 10:45 259** Biophysical characterization of *Ostrinia nubilalis* olfactory protein: An eco-friendly approach to disrupt insect mating. **V. Nukala**, O. Al-Danoon, S. Ayyappan, S. Mohanty
- 11:03 260** Conformational dynamics and supertertiary interactions within PDZ3-SH3-GuK core supramodule of PSD-95 postsynaptic scaffolding protein. **N. Saikia**
- 11:28 261** Modulating amino acids in different regions of Cas12a for error-proof genome tools. **L. Martin**, R. Rajan
- 11:44 262** Co-assembly of alpha-helical peptides into higher order fibers. **O. Abualsoud**

Chemical Production at Industrial Scale

Omni Oklahoma City Hotel, Oklahoma Station 2

M.S. Rosen, C. Varnado, *Organizers, Presiding*

- 8:00** Introductory remarks.
- 8:10 263** Chemicals and cars: Back to the future. **C. Varnado**
- 8:40 264** Industrial scale sulfur chemistry and its use in producing compounds vital to modern society. **C. Brown**
- 9:10 265** Sulfur – a key element that might see significant long-term supply disruptions: Background, outlook and implications. **B.P. Grady**
- 9:40** Break.
- 10:00 266** Coatings products and solutions for the old and gas industry. **A. Paul**

10:30 267 Troubleshooting commercial production of bromine derivatives. **J.T. Aplin**

11:00 268 Vinyl chloride: Two hemispheres, two processes. **W.F. Carroll**

Functional Inorganic Materials

Omni Oklahoma City Hotel, Oklahoma Station 7

Cosponsored by COLL

Financially supported by J. Luminescence Materials Advances

J. Chan, B. Saparov, *Organizers*

Y. Vasquez, *Organizer, Presiding*

J.G. Tischler, *Presiding*

8:00 269 Nanoimaging of chemical heterogeneity with sub-wavenumber frequency resolution. **T.G. Habteyes**, W. Takele

8:25 270 Photoluminescence in atomically precise, thiolate-stabilized nanoclusters. **C.M. Aikens**, S. Havenridge

8:50 271 Cellular uptake and cytotoxicity of varying aspect ratios of gold nanorods in HeLa cells. **Y. Vasquez**, D. Fernando, S. Sulthana

9:15 272 High temperature in situ powder X-ray diffraction for metal flux growth synthesis of praseodymium cobalt germanides. **T.M. Kyrk**, S.H. Lapidus, J. Chan

9:35 273 Synthesis, structure determination, and physical properties of $Ba_2InSnPn_3$ ($Pn = P, As$) Zintl phases. T. Kandabadge, S. Bobev, **S. Baranets**

10:00 Break.

10:20 274 Tailoring 1D exciton coherence in crystalline small molecules thin films. **M. Furis**, L. Liang, V. Mapara, S. Raybould, L.A. Bumm

10:45 275 Quantifying the energetics of thermally activated up-conversion in $CsPbBr_3$ perovskite nanocrystals: Implications for optical cooling. **M.T. Sheldon**

11:10 276 Biexciton recombination dynamics in single strongly confined perovskite quantum dots. **Y. Dong**, C. Mi, G. Gee, M. Atteberry

11:35 277 Dimensional enhancement and reduction in ns^2 pnictogen halides: Design principles for self-trapped exciton emission. **K. McCall**

Inorganic: Photochemistry and New Ligand/Complex Design

Omni Oklahoma City Hotel, Route 66

R. Latifi, L. Tahsini, *Organizers*

D.M. Jenkins, *Presiding*

8:00 472 Bimetallic main-group catalysts for the synthesis of biodegradable polymers. **P. Naik**

8:20 279 Synthesis, characterization and photophysical studies of low-coordinate Cu(I) complexes bearing diaminocarbene ligands. **C. Hunt**, L. Tahsini

8:40 280 Synthesis and characterization of tri-dentate quinoline-based OCN ligands and their complexes. **N. Noei**, J. Rein, L. Tahsini

9:00 281 Design and synthesis of pnictogen cages for pnictogen bond driven self-assembly of reversed bilayer vesicles for aqueous environments. **L.M. Delgado**, A.F. Cozzolino, S. Yeh

- 9:20 Break.
- 9:40 282 Interactions of arylhydroxylamines and alkylaldoximes with a rhodium porphyrin. **J. Londoño-Salazar**, M.A. Ayala, D. Powell, Y. Shao, G.B. Richter-Addo
- 10:00 283 Controlling metal organic nanotube (MONT) formation through improved design of di-1,2,4-triazole ligands. J.A. Barrett, P. Nalaoh, N.D. Rosenmann, N.C. Gianneschi, **D.M. Jenkins**
- 10:20 284 Synthesis, characterization, and biological activity of novel organoantimony(V) cyanoximates. K.A. Pinks, **N. Gerasimchuk**, M. Patrauchan
- 10:40 285 Self-assembly and characterization of low spin Fe(II) complexes of tridentate mixed amine/imine ligands with both cis- and trans-1,2-cyclohexanediamine backbones. **C.B. Hollandsworth**, N. Gerasimchuk
- 11:00 286 Convenient synthesis and bioactivity studies of picoplatin derivatives. **Q. Zhao**
- 11:20 287 Nonsymmetrical linkers for the design of metal organic frameworks with hybrid properties. **T. Ericson**, B. Agarwal, A.F. Cozzolino
- 11:40 288 New polypyrazoleborate complexes of iron(II). **A. Oberley**

Solar, Fuel, Wind and Future Energy

Omni Oklahoma City Hotel, Oklahoma Station 1

L. Ford, *Organizer*

W. Wei, *Presiding*

- 8:00 289 Enhancements in convective self-assembly: Defect reduction and novel binary colloidal patterning. **S. Das**
- 8:20 290 Hydrophobic carbon nanosheets for perovskite solar cells. **W. Wei**
- 8:40 291 Effect of plasmonic energetic electrons on chemical reactions. **T. Le**, T. Salavati-Fard, B. Wang
- 9:00 292 Investigation of hot carriers in highly stable $\text{FA}_{0.8}\text{Cs}_{0.2}\text{Pb}_{1.02}\text{I}_{2.4}\text{Br}_{0.6}\text{Cl}_{0.02}$ perovskite solar cells. **H. Afshari**, V. Mapara, M. Khanal, V. Whiteside, R. Scheidt, M.C. Beard, G. Eperon, M. Furis, I. Sellers
- 9:20 293 Effect of carbon dot on photovoltaic performance of n-TiO₂/p-NiO heterojunction in dye-sensitized solar cells. **T.F. Yadeta**, I. Toyoko
- 9:40 Break.

Sustainability and Recycling of Materials

Omni Oklahoma City Hotel, Oklahoma Station 6

H. Cheng, R. Vaidyanathan, *Organizers, Presiding*

- 8:00 Introductory remarks.
- 8:05 294 Selective catalytic upgrading of multilayered films. D. Bui, H.K. Chau, S. Abdolbaghi, Q. Nguyen, L. Trevisi, B. Wang, L. Lobban, **S. Crossley**
- 8:30 295 Sustainable, degradable, and recyclable polymers derived from cyclic disulfides. **N.V. Tsarevsky**

- 8:55 296** Sustainable resin design for 3D photoprinting. **R. Smaldone**
- 9:20 249** Structural composites from post-consumer used poly(ethylene terephthalate) (PET) carpet with recycled polypropylene (PP) resin. **L. Kamran**, R. Azarfam, F.D. Blum, R. Vaidyanathan, J. Hanan
- 9:40 298** Training for improving plastics circularity in the Plastics Engineering Technology program at Pittsburg State University. **J.H. Norton**, G. Murray, P. Herring, D. Spielbusch
- 10:05** Break.
- 10:25 299** Vegetable oil-based polymers and composites prepared in green media. **Z. Liu**
- 10:50 300** Recycled polymer composites from mixed polymer blends and graphene oxide. **T. Meadows**, S. Chaudhari, R. Vaidyanathan
- 11:10 301** Composite coextruded using recycled polymers reinforced with discarded carpet. C. Scott, J.C. Hanan, **M. Allahkarami**, S. Chaudhari, C. Switzer, R. Vaidyanathan, F.D. Blum
- 11:30 302** Applications of cellulose nanomaterials from cotton ginning byproducts. **J.H. Jordan**, M.W. Easson

Best Practices for Successful Small Chemical Businesses

Omni Oklahoma City Hotel, Bricktown

G. Garrison, *Organizer*

D.W. Smith, *Presiding*

- 8:20 303** The influence of corporate governance on financial reporting quality in the Taiwan chemical and paint industry. **L.A. Geleta**
- 8:40 304** Advancing chemical education and navigating success for a small business, Mega Molecules, LLC. **C. Hirtzel**
- 9:00 305** There's plenty of room at the bottom: The case for small businesses in the greater chemical enterprise. **P.J. Bonk**
- 9:20 306** Tetramer Technologies: A case study for faculty startup navigation and exposing the "win-win" in nascent cultures of university entrepreneurship. **D.W. Smith**
- 9:40** Break.
- 10:00 307** The creation of lasting successful chemical businesses in Oklahoma, the legacy of Dr. Allen Ablett. **N.F. Materer**
- 10:30 308** Plants to plastix: Sustainability eco-system business models and rethinking how we use our natural resources. **S. Perry**
- 10:50 309** Dry surface technology and innovative superhydrophobic solutions. **S. Kennedy**
- 11:10 310** Hand Technologies: Bridging academia and entrepreneurship to the graduate student landscape. **E. Borrego**, W. Johnson, J. Brown, P. Madden, C.U. Pittman, D.W. Smith
- 11:30 311** Operational challenges for dry blending materials: Successful small chemical business. **G. Garrison**

Cope Scholar Symposium: Enabling Approaches to Chemical Synthesis

Omni Oklahoma City Hotel, Oklahoma Station 3

Cosponsored by ORGN

J. May, J.D. Weaver, *Organizers, Presiding*

- 8:20 312** Contrathermodynamic catalysis: An attempt to develop synthetic photosynthesis.
J.D. Weaver
- 8:50 313** Reimagining ancient reactions for the 21st century. **A.A. Thomas**
- 9:20 314** Chemical investigations inspired by structurally unusual alkaloids. A. Morrow, F. Xu, J. Aquilina, A. Banerjee, **M. Smith**
- 9:50** Break.
- 10:10 315** Asymmetric synthesis leveraging alkenyl boronates. **J. Ready**
- 10:40 316** Catalytic C-C coupling of alcohols via hydrogen auto-transfer: Reinventing carbonyl addition. **M.J. Krische**
- 11:10 317** Synthesis of the masked acyl cyanide, TBS-MAC, and its application as an oxidation state three synthon. **J.A. Pigza**

Biochemistry Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

O. Prakash, *Organizer***9:00 - 11:00**

- 318** H-loop residues in glutathione synthetase. **L. Dollar**, J. Gruber, L. Haynes, H. Conrad-Webb, M.E. Anderson
- 319** NMR structural studies of an insect cytokine. **A. Su**, H. Miller, N. Mishra, T. Kimura, H. Jiang, O. Prakash
- 320** Characterization and activation of *Manduca sexta* stress responsive peptides. **B. Arria**, A. Su, T. Kimura, X. Cao, Y. Wang, H. Jiang, O. Prakash
- 321** Inhibition of ovarian cancer proliferation: Targeting oxysterol-binding proteins and intracellular lipid transport. **R.H. Bui**, J.L. Berrios-Rivera, S. Nimmo, A.W. Burgett
- 323** Repurposing an anti-tumor drug candidate for targeting bacterial ATP-dependent proteases. **Z. Spaulding**, S. Shiva, C.B. Ranweera, M. Zolkiewski
- 324** Polymorphism of OHet72 nanocrystals: Impact of solvent on nanocrystal formation. **A.K. Beathard**, L. Garcia-Contreras
- 325** Association between RND efflux pumps and bacterial physiology in *Pseudomonas aeruginosa*. **L. Ajmal**, H.I. Zgurskaya
- 326** Unveiling precision targets: OSBP and ORP4 in ovarian cancer therapy with OSW-1 analog compounds. **S. Choudhary**, R. Bui, J.L. Berrios-Rivera, S. Nimmo, A.W. Burgett
- 327** Development of a novel algorithm to recognize palindromes within proteins. **J. Garner**
- 328** New tools for studying diabetic retinopathy: Identifying and quantifying pericytes and endothelial cells in the mouse retina. **Q. Yan**
- 329** Determining oxysterol-binding protein (OSBP) structure and function to guide drug development. **R. Bayimenye**, J.L. Berrios-Rivera, S. Nimmo, C.R. Bourne, A.W. Burgett

Catalysis and Energy: Inextricable Links in the Chain of Progress Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

S. Crossley, J.L. White, *Organizers*

9:00 - 11:00

- 330** Electrochemical behavior of binder-free cobalt phosphate for supercapacitor and water splitting applications. **H. Chaudhary, R.K. Gupta**
- 331** Hierarchical design of rhodium selenide nanostructure as high-performance trifunctional electrocatalysis for water splitting and oxygen reduction. **H. Singh**, M. Nath
- 332** Improving the electrochemical properties of MnO₂ by doping with Fe for water splitting and supercapacitor application. J. Okwe, **R.K. Gupta**
- 333** Boron nitride supported atomically dispersed transition metal dimers for electrochemical nitrogen reduction. **V. Choutipalli**, U. De Alwis, K.L. Shuford
- 334** Synthesis of iron oxide as an efficient electrocatalyst for water splitting application. **N. Maley**, P. Patel, **R.K. Gupta**
- 335** Carbon nanotubes as hydrogen highways: Deciphering hydrogen spillover in reduction oxide catalysts. **T.E. Zhang**, C. Bavinaka, L.A. Gomez, S. Crossley
- 336** Synthesis, studies of naphthoquinone, anthraquinone derived iridium pincer catalysts for ethanol to butanol conversion. **A. Rahman**, W.D. Jones

Computer Simulations of Biochemical Processes: From Quantum to Classical and Back Again Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

M. McCullagh, *Organizer*

G.A. Cisneros, *Organizer, Presiding*

H. Torabifard, *Presiding*

9:00 - 11:00

- 337** Bridging protein dynamics and catalysis: Exploring lid domains in adenylate kinase. **A. Arattu Thodika**, K. Nam
- 338** Combining anharmonic corrections with SQM Pulay style scale factors to improve molecular vibration predictions. J. Moon, **W.B. Collier**
- 339** Mechanisms of DNA cleavage in CRISPR-Cas systems. **R. Van**, X. Pan, J. Liu, P.K. Agarwal, R. Rajan, B. Brooks, Y. Shao
- 340** Investigating crosstalk between H2A ubiquitylation and H3K36 methylation through molecular dynamics simulation of histone-N-methyltransferase. **T. Shah**, H. Torabifard
- 341** A matrix isolation and vibrational study of 19 K argon matrix isolated 5-fluoro-2'-deoxyuridine. **W.B. Collier**, S. Lee, K.H. Sang, G. Ritzhaupt, C. Klehm, P. Desmon
- 342** Ensemble mechanism of allostery in rabbit muscle pyruvate kinase. **R. Marahatha**, M. McCullagh
- 343** Creative component report on spherical mapping of intermolecular interactions (SHIM BUILDER). **H. Mozafarimanesh**, C. Fennell, S. Darapureddy

- 344 On the role of the gamma-Zn(II) in the hydrolysis of phosphate esters by PHP. **D.P. Linder**, A. Linder, A. Bigley
- 345 Modeling water by enforcing ideal liquid behavior. **Y. Wijesiriwardena**, C. Fennell
- 346 Mechanistic insights of Leu405Asp mutation in ATP Pocket of Nsp-13 helicase from molecular dynamics simulations. **K. Frederick**, P. Roy, M. McCullagh
- 347 Multiscale simulations of the thermal isomerization of molecular photoswitches in biomolecular environments: Insights into reaction pathways and protein binding effects. **A. Bakhtiari**, G.J. Costa, R. Liang

Design, Synthesis, and Characterization of Functional Polymeric Materials Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

Cosponsored by POLY

C.E. Callmann, E. Pentzer, *Organizers*

9:00 - 11:00

- 348 High-performance iodine adsorption in amide functionalized two-dimensional covalent organic frameworks. **N. Arora**, T. Debnath, G.A. Cisneros, R. Smaldone
- 349 Magnify bonding strength: Development and characterization of epoxidized soybean oil-based adhesive resin. **J. Patel**, U. Panchal, P. Patel, **R.K. Gupta**
- 350 Influence of pure and reused canola oil based on the structural and thermomechanical properties of rigid polyurethane foams. **J. Patel**, P. Patel, **R.K. Gupta**
- 351 Synthesis of novel vegetable oil-based polyol and the effects of melamine, dimethyl methyl phosphonate, and melamine salt (DPPMA) on the properties of rigid polyurethane foams. **J. Chaudhari**, P. Patel, **R.K. Gupta**
- 352 Hybrid hydrogels crosslinked with dynamic thiol-Michael and non-dynamic thiol-maleimide bonds for controlled drug release application. **K. Thapa**, E. Torres, T. FitzSimons, M. Otakepor, M. Siller, A. Crowell, A. Rosales, T. Betancourt
- 353 Post polymerization modification of polyacrylamides through amide activation. **K. Wekasinghe**, N.L. Manny, E.R. Walther, A. Teator
- 354 Towards a rearrangement-mediated chain growth polymerization. **A. Lininger**, A. Teator
- 356 Halogen-free flame-retardant rigid polyurethane foam using non-edible oil-based polyol. **N. Chaudhary**, P. Patel, **R.K. Gupta**
- 357 High-performance flame-retardant polyurethane foams: Effect of flame retardants on the properties. **S. Kondaveeti**, P. Patel, **R.K. Gupta**
- 358 Soybean oil-based adhesives: Effect of amines and processing time. U. Panchal, J. Patel, P. Patel, **R.K. Gupta**
- 359 Non-isocyanate polyurethane film from carbonated soybean oil with aliphatic diamines. **P. Patel**, **R.K. Gupta**
- 360 Sequestration of brilliant green from aqueous solution using composites of reduced graphene oxide with chitosan and chitosan beads: Experimental and computational studies. **O. Oluwasina**, A. Adedeji, S. Olusegun, O. Oluwasina

- 362** Surface functionalization of 3D printed metal organic framework composites. **R. Johnson**, S. Pererra, R. Pawle, T. Tran, L. Ayers, V. Ganesh, M. Senarathna, K.P. Cortes-Guzman, S. Doube, S. Springfield, L.F. Hancock, B.R. Lund, R. Smaldone
- 363** Synthesis and characterization of high molecular weight branched poly(pentylene adipate-co-terephthalate). **H. Aboukeila**, O. Singh, J. Klier, B.P. Grady
- 365** Analyzing a degradable natural polymer-based novel wound dressing for use in biomedical applications. **W. Lawrence**, S.K. Hamilton
- 366** Electropolymerization and characterization of polyphenol coatings for the corrosion protection of mild steel. **J.M. Etheridge**, E. El-Giar
- 367** Biobased copolyesters poly(pentylene dodecanoate-co-furandicarboxylate): Synthesis, characterization, and thermo-mechanical properties. **O. Singh**, H. Aboukeila, B.P. Grady, J. Klier
- 369** Synthesizing a novel wound care fiber mat and testing its hemostatic properties capabilities. **C.M. McClain**, S.K. Hamilton

Diversity in Chemistry and STEM Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

M.F. Borunda, K. L. Johnson-Winters, *Organizers*

9:00 - 11:00

- 370** Midwestern State University ACS student affiliates: DEI community projects. C. Fulton, **A. Vann, K. Davis, A. Simbana**
- 371** Building engagement in laboratories, networking, and peer groups: BELONG in STEM Scholars Program to increase student diversity at Northern Illinois University. **R.A. Wheeler**, T. Hagen, N. LaDue, T. Reeves, D. Dugas

Illicit Fentanyl: A Perfect Storm in Science Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

D.J. Nelson, A.M. Timmons, *Organizers*

9:00 - 11:00

- 372** Fentanyl in recent news. **D.J. Nelson**
- 373** Fentanyl and the devastating effects on students and young adults: Statistics and current status. **D.J. Nelson**
- 374** Growing threat of illicit fentanyl in the United States. D.J. Nelson, **C.C. Collier, J. Macias, C. Gormley**
- 375** Solid-phase extraction of fentanyl analogs in biological matrices for analysis by LC-MS/MS. **A.M. Timmons**

Physical Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

E. Schnitzler, Y. Shao, *Organizers***9:00 - 11:00**

- 376** Investigation of photophysics of fluorescent Texas Red dyes in confined environment. **D. Kim**, N. Moro, R. Nayak
- 377** Creating potential energy surfaces on the fly, using the Crystal code. **M. Aarabi**, A. Pandey, B. Poirier
- 378** Carbon dioxide disassociation through the use of ceria-based catalysts. **D. Acker**, P. Mynarski, S. Kumar
- 379** Laboratory and pharmaceutical aerosol generators may also be generating trace amounts of hydrogen peroxide. **S.M. Liyanage**, E. Schnitzler
- 380** Chalcogen bond interactions as catalytic mediators for aromatic sulfur oxidation in petroleum desulfurization. **K.A. French**, K.L. Shuford
- 381** Characterization of functionalized and non-functionalized carbon nanotubes and their exposure to carbon dioxide and solvents. **D. Woodring**, J. Paniagua, J.D. Beatty, N. Mirsaleh-Kohan
- 382** Kinetics of an intramolecular PCET reaction under extreme pressure. **S. Watson**, H. Yan, P. VanNatta
- 383** Cavity quantum electrodynamical time-dependent density functional theory within gaussian atomic basis for excitonic polariton states of many-molecule system. **Z. Pei**, J. Yang, Q. Ou, Y. Shao
- 384** Distance of detection: A σ -hole study. **D. Devore**, T.L. Ellington, K.L. Shuford
- 385** Biomass burning organic aerosol from tallgrasses on the Great Plains: Hygroscopicity, absorbance, and the role of charge-transfer complexes in fresh and aged brown carbon from summer and winter grasses. **C. Calvert**, K.L. Betz, E. Bruce, E. Schnitzler
- 386** The effect of rigidity on properties of flexible water models. **R. Weldon**, F. Wang
- 387** Pressure modulated monoxidation of C-H bonds by dicopper-m-oxo complex. **N. Martell**, P. VanNatta, H. Yan
- 388** Photophysical and hydrodynamic studies of fluorescent dye AF647 in presence of graphene oxide nanocolloid. **N. Moro**, W. Johnson, D. Kim, R. Nayak
- 389** Interactions and rotational correlation times of ionic liquid and its binary mixtures with methylimidazole. **S. Sagala**, E.L. Quitevis, J. Kaur
- 390** High-throughput computational screening of MO₂ transition metal oxides as efficient oxygen electrocatalysts for green hydrogen production. **S. Navodye**, A. Sison, K. Gunasooriya

Analytical

Omni Oklahoma City Hotel, Oklahoma Station 1

S. Gamagedara, *Organizer, Presiding*

- 10:05 391** Monitoring per- and polyfluoroalkyl substances in Central Arkansas surface waters. **A. Treadway**, J. Nolen, G. Boysen

- 10:25 392** ETL 5D SPORT in resolving intracellular transport of nano cargo in live cell. **M. Yang**, J.E. Batey, B. Dong
- 10:45 393** Chemical discrimination of multiple phenolic acids with a cyclodextrin supramolecular host. X. Yao, **M. Bonizzoni**
- 11:05 394** Extracting targeted quantitative proteomics data from data independent acquisition. W. Landrith, H. Landrith, B. Loveland, C. Kinter, **M. Kinter**
- 11:25 396** Electrochemical detection of active pharmaceutical ingredients in over-the-counter medications using screen-printed-electrodes. **M. Massoud**

THURSDAY AFTERNOON, November 16, 2023

Analytical

Omni Oklahoma City Hotel, Oklahoma Station 1

S. Gamagedara, *Organizer, Presiding*

- 1:00 397** Classification and characterization of brown seaweed species using differential sensing and LC-MS. **R. Patel**, D. Zamora-Olivares
- 1:20 398** Ovarian cancer biomarker profiling with pyrenyl-nanocarbon antibody arrays. **Z. Syed**, S. Krishnan, D. Benbrook
- 1:40 399** Spectroscopic investigation of Maya pottery sherds from Guatemala. **M.J. McFarland**, K.K. Onchoke
- 2:00 400** Determination of pKa's in glycine-metal complexes under protic solvent conditions by spectroscopic methods. **J. Henrikson**
- 2:20 401** Doxorubicin-based Chemo-PTT combination nanomedicines. **N. Siraj**
- 2:40** Break
- 3:00** Break.
- 3:20 403** Method adaptation and optimization of three common analytical techniques for environmental sampling and analysis of nicotine from electronic cigarette emissions. **T. Oni**, E. Floyd, S. Gamagedara
- 3:40 404** Allergen proteome profiling and quantitation of Oklahoma grass species. **S. Gamagedara**, E. Dowd, N. Ahsan
- 4:00 405** MassLite: An easy-to-use single cell mass spectrometry data pretreatment platform based on python. **Z. Zou**, Z. Yang
- 4:20 406** Colorimetric determination of chromium (VI) in water. **A. Iob**

Biochemistry: Macromolecular Structure and Function

Omni Oklahoma City Hotel, Myriad

R. De Guzman, *Organizer*S. Mohanty, *Organizer, Presiding*E.D. Holmstrom, *Presiding*

- 1:00** Introductory remarks.
- 1:10 407** The awesome power of fluorine NMR – from drugs to cells. **A.M. Gronenborn**
- 1:50 408** Inward-rectifier K⁺ channel transmembrane and positive lipid-loading allostery observed by solid-state NMR. **B. Wylie**
- 2:15 409** Understanding the impact of mucin as surface-active molecules on the interfacial rheology of salivary droplets. **E. Barros de Oliveira**, S. Razavi
- 2:35 410** Integrated structural model linking palladin to actin dynamics. **M.R. Beck**
- 3:00** Break.
- 3:20 411** Novel mechanism of pheromone release in *Ostrinia Furnacalis*. **S. Ayyappan**, P. Combs, S. Mohanty

- 3:40 412** Role of phenyl butyrate as a chemical chaperone in the regulation of misfolded alpha-synuclein fibrils. **K.A. Baffour**, T. Banerjee
- 4:00 413** Computational studies of human STING: Effects of binding small molecules. H. Gates, S. Crivelli, **M. Watanabe**
- 4:20 414** Dual fluorescence of natural flavonoid kaempferol in quadruplex DNA matrix. **B. Sengupta**

Chemical Production at Industrial Scale

Omni Oklahoma City Hotel, Oklahoma Station 2

M.S. Rosen, C. Varnado, *Organizers, Presiding*

- 1:00** Introductory remarks.
- 1:05 415** Navigating the hurdles of industrial chemical manufacturing in 2023. **A.S. Hinkle**
- 1:35 416** Practical challenges of economic production of modern polyolefins. **D. Ginger**
- 2:05 417** Commercial selective 1-hexene/1-octene catalyst development. **O.L. Sydora**
- 2:35 418** Chromium-based catalysts with phospholane ligands for ethylene tetramerization. **M.S. Rosen**
- 3:05** Break.
- 3:25 419** Catalyst development for ethylene oxide production: Innovation of METEOR™ EO RETRO catalysts. **D. Jain**
- 3:55 420** Styrenic block copolymers in a sustainable future – going from petroleum to renewable sources and enabling a sustainable polymer economy. **D.S. Germack**

Cope Scholar Symposium: Enabling Approaches to Chemical Synthesis

Omni Oklahoma City Hotel, Oklahoma Station 3

Cosponsored by ORGN

J. May, J.D. Weaver, *Organizers, Presiding*

- 1:00 421** Skeletal photo-isomerization as a key tool for the exploration of new chemical space. **Z. Boskovic**
- 1:30 422** Programmed carbocyclizations of conjugated polyenes. **J. Frederich**
- 2:00** Break.
- 2:20 423** Fluorogenic polymer synthesis for signal amplification and biodetection. **C.B. Cooley**
- 2:50 424** Harnessing carbene/nitrenes for drug discovery. **I. Sharma**
- 3:20 425** Asymmetric functionalization of sulfonimidamides guided by chemical space analysis. **N. Lim**
- 3:50 426** New avenues in synthesis via organic photoredox catalysis. **D.A. Nicewicz**

Organic

Omni Oklahoma City Hotel, Bricktown

R.R. Kane, *Organizer, Presiding*

- 1:00 427** Phenolic acids as binding probes for cyclodextrin complexation. X. Yao, **M. Bonizzoni**
- 1:25 428** Fluorescent chemosensing spiropyran-based molecules and materials for gas phase ion detection. **R.L. Miller**, P.D. Williams, A. Carlson, B. Jones, F.W. Foss
- 1:45 429** Analyzing the accuracy of critical micelle concentration predictions using deep learning. **A.W. Moriarty**, T. Kobayashi, M. Salvalaglio, P. Angeli, A. Striolo, I. Mcrobbie
- 2:05 430** Heavy metal sensing calix[4]arene derivatives and the detection of neutrinoless double beta decay. **R. Madigan**, W. Gerro, P. Nino, B. Jones, F.W. Foss
- 2:25 431** Synthesis of carbonyl-functionalized ladder-type oligo(*p*-phenylene)s for probing electron delocalization. **R. Peri**, J. Yan
- 2:50** Break.

Physical 3

Omni Oklahoma City Hotel, Route 66

E. Schnitzler, *Organizer*Y. Shao, *Organizer, Presiding*R. Wheeler, *Presiding*

- 1:00 432** Mechanistic insights into cobalt-catalyzed Fischer-Tropsch synthesis. **K. Gunasooriya**
- 1:20 433** Cognizance of QD van der Waals heterostructures: An in-depth DFT study of properties and electrochemical applications. **U. De Alwis**, V. Choutipalli, K.L. Shuford
- 1:40 434** Developing structure-function relationships for the design of optoacoustic imaging probes. **C. Wickizer**, W. MacCuaig, R. Van, Y. Shao, L. McNally
- 2:00 435** Hybrid and mixed basis sets strategies for water cluster XPS calculations. **A. Delgado**, D. Matthews
- 2:20 436** Understanding the effects of acid electrolyte anions on IrO₂ for oxygen evolution reaction. **S. Navodye**, K. Gunasooriya
- 2:40 437** Density functional theoretical studies of mononitrated chrysenes. **K.K. Onchoke**
- 3:00** Break.
- 3:20 438** Spatial signatures of electron correlation in least-squares tensor hypercontraction. **C. Yin**, S. Becker, J. Thorpe, D. Matthews
- 3:40 439** Chemical warfare agent hydrolysis in the NU-1000 Zr-MOF: Structure, topology, and the impact of humidity. **M. Oliver**, L. Huang
- 4:00 440** Robust least squares tensor hypercontraction for the particle-particle ladder term in EOM-CCSD. **A. Datar**, D. Matthews
- 4:20 441** DFT study of selective alkane halogenation by non-heme iron catalysts: Evidence for Fe^v(acacen)(oxo)(halide) as an active intermediate. **W.M. Dagnaw**

Sustainability and Recycling of Materials

Omni Oklahoma City Hotel, Oklahoma Station 6

H. Cheng, R. Vaidyanathan, *Organizers, Presiding*

- 1:25 443** Mechanistic insight to generating hexane from cellulose using hydrogen bronze materials. **D.W. Scott**
- 1:50 444** Investigation into the reaction pathways and catalyst deactivation for polyethylene hydrogenolysis over silica-supported cobalt catalysts. **S. Borkar**, R. Helmer, S. Panicker, M. Shetty
- 2:10 445** Use of agro-based materials for sustainability research and development. **H. Cheng**, A. Biswas
- 2:35** Break.
- 2:55 446** Fabrication and application of portable batteries based on recyclable and household materials. **M. Jiang**, K. Patino, M. Parker
- 3:20 447** Glass half full: Glass recycling for coastal restoration and more. **J. Vanegas**, F. Trautmann
- 3:45 448** Sorbent for environmentally friendly treatment of agriculture runoff. **C. Kelley**
- 4:05 449** Mg²⁺/Al³⁺ layered double hydroxide synthesis for phosphate and nitrate removal from aquatic environments. **P. Kitzel**
- 4:25 442** Creating a sustainable food future by 2050 via systems engineering approaches. **Z. Jiang**, Z. Song

Functional Inorganic Materials

Omni Oklahoma City Hotel, Oklahoma Station 7

Cosponsored by COLL

Financially supported by J. Luminescence Materials Advances

J. Chan, B. Saporov, *Organizers*

Y. Vasquez, *Organizer, Presiding*

J.G. Tischler, *Presiding*

- 1:35 451** Optimizing the reactivity of Ti₂N MXene through decoupling surface and bulk structure and phenomena. R. Yoo, D. Johnson, **A. Djire**
- 2:00 452** Understanding the fundamentals of heterogeneous catalysis for energy-relevant chemical transformations. **H. Noh**
- 2:20 454** Enhanced infrared photodiodes based on PbS/PbCl_x core/shell nanocrystals. A. Colbert, D. Placencia, E. Ratcliff, J.E. Boercker, P. Lee, E. Aifer, **J.G. Tischler**
- 2:45** Break.
- 3:05 455** Advancing synthesis and structure-property relationships of semiconducting mixed anion materials. **H. Nguyen**, R.T. Macaluso
- 3:30 456** Single-molecule imaging of photocatalytic dynamics in nanomaterials. **B. Dong**
- 3:55 457** From energetic materials to functional materials: Synthesis of cobalt single-atom catalysts on carbon. **J. Yan**, X. Zhang, X. Wang, P. Chen, Y. Zhao
- 4:20 724** Chiral symmetry emerges during the self-assembly of tetrahedra. **M.R. Jones**

Chemical Education Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

J. Mutambuki, *Organizer***2:00 - 4:00**

458 LibreText OER for the general chemistry lecture and laboratory. **R.E. Belford**, L. Poirot, E. Waters

459 Get involved with the ACS Division of Chemical Education. **S.G. Prilliman**

Inorganic Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

R. Latifi, L. Tahsini, *Organizers***2:00 - 4:00**

460 Development of copper containing nitrite reduction electrocatalyst for water purification. **V. Hulse**, K. Knecht, N. Elgrishi

461 Assessing hydrogen bonding effects in concerted proton-electron transfer reactions using Mn^{III}-methoxy complexes. **G.J. Graf**, S.A. Brunclik, P. Singh, A.A. Opalade, T.A. Jackson

462 Greener approach to synthesis of novel copper(I) and silver(I) complexes with caffeine by comparison of solventless reaction via mechanical grinding and solvent-mediated reaction via Schlenk line technique. **B. Hitt**, S. Banna, Z. Taimuri, E. Burley, M. Rawashdeh-Omary

464 Fluoro-bridged Tb-MOFs via defluorination of PFAS. **S. Sheybani**, M. Joy, K.J. Balkus

465 A second pyridine ring and 4-position substitutions improve the catalytic reactivity of Fe-pyridinophane complexes. **K.J. Smith**, J. Bonnell, K.N. Green

466 Synthesis, X-ray, and theoretical structural analysis of a binuclear manganese tricarbonyl thionicotinic acid complex. **A. Rahman**, D. Hossain

467 Several new lanthanide metal-organic frameworks exhibiting fluoro-bridged trinuclear clusters and their magnetic and luminescence properties. **M. Mortensen**, M. Abbas, G. McCandless, K.J. Balkus

468 Structures and reactivity of cobalt hydride complexes containing tridentate and monodentate phosphine complexes. **A.E. Robinson**, C. Zall

469 Neutral antimony(V) Lewis acids for the transport of fluoride across phospholipid membranes. **B. Murphy**, L. Maltz, F.P. Gabbai

470 Characterizing interactions between a tetrahedral metal-organic cage and electrocatalysts for CO₂ reduction. **J. Grundhoefer**, R. Bujol, J. Bruna

471 Copper(II) L-histidine complexes and their derivatives containing carbonyl groups, novel crystal structures, characterization, and electrochemical properties. **G.M. Chiarella**, C. Cash, D. Toole, H.N. Herath

473 Introducing green chemistry in undergraduate laboratory: Catalytic oxidation of anthracene in aqueous biphasic medium. P. Siemens, E. Coronado-Franco, I. Baker, C. Brewer, **C.A. Mebi**

474 Uranyl bending: Inductive effects on the bond strength of uranyl (UO₂²⁺) ions. **D. Eralie**, E.A. Hiti, D.T. Bhakta, J.A. Williamson, J.D. Gorden, S. Vasylevskyi, A.E. Gorden

- 717** Synthesis and characterization of new tetradentate bis(pyridinecarboxamide)-benzene (non-heme) Ru(II) nitrosyl complexes: Comparisons between the heme and non-heme systems. **T.A. Kapfunde**, G.B. Richter-Addo

Materials/Polymer Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

N. Green, R.K. Gupta, *Organizers*

2:00 - 4:00

- 475** Graphene, graphene oxide, boron oxide for space suits applications: A first-principle investigation. **S. Lang**, S. Lin
- 476** Self-assembling peptides with internal ionizable non-natural amino acids: A new approach to pH-responsive peptide materials. **H. Asokan Sheeja**, S. Yang, H. Dong
- 477** Environmental consideration of chlorhexidine interaction with cellulose. S. Huynh, **D. Brown**, **J.D. Beatty**
- 478** Synthesis, functionalization, and characterization of ssDNA coated dye-doped silica nanoparticles. **S. Sharpe**
- 479** Direct analysis of aldehydes and EPA TO-11 compounds on diffusive passive chemical vapor samplers. **Z. Brown**, E. Kadossov, M.L. Teicheira, N.F. Materer, A.W. Aplett, S. Shaikh

Organic Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

R.R. Kane, *Organizer*

2:00 - 4:00

- 480** Synthetic utility of laughing gas. **D. Herndon**, **J. Solomon**, S. Singh, I. Sharma, K.M. Nicholas
- 481** Efforts toward the total synthesis of phorbosone A. **K. Lee**, T. Peterson, E.E. Osborn, A. Dowell
- 482** Flow synthesis and cancer cell cytotoxicity of caffeic acid phenethyl amide (CAPA) derivatives. A. Saucedo, N. Mesa-Diaz, J. Smith, A. Vernaza, I. Du, **S.M. Kerwin**
- 483** Synthesis and evaluation of *n*-alkylated derivatives of 2-amino-4,6-diphenylpicolinonitrile as potential anticancer agents against breast cancer cell lines. **A.R. Al-Ghamdi**, R.I. Al-Wabli, M.S. Almutairi, A.M. Rahman
- 484** Synthesis and evaluation of unnatural prodigiosin analogs as anti-cancer drugs. **J. Alley**, B. Walker, S.V. Jenkins, R.J. Griffin
- 485** Synthesis and characterizations of carbonyl-functionalized indenofluorene. **J.O. Ehoche**, J. Yan, R. Peri
- 486** Synthesis, purification, and characterization of guest molecules in cucurbit[n]urils. **R. Webb**, S. Ellis
- 487** Synthesis of tricyclic and tetracyclic imidazole-containing heteroarenes. **N. Khanal**, J.L. Bolliger
- 488** Synthesis of ether and amine functionalized cholesterol derivatives for use in metal-complex based imaging agents. D.A. Nilson, **D.E. Martyn**

- 489 Synthesis of selenium containing heterocycles. **S. Thapa**, J.L. Bolliger
- 490 Synthesis and electrochemistry results of aryl substituted methylene malonates. **G. Linthicum**, **S. Ibarra Chavez**, C.A. Hansen
- 491 Stereoselective domino Michael-Henry reaction of 1,2-cyclohexanedione with nitroolefins catalyzed by an amino acid-Ni(acac)₂ complex. **B.N. Nguyen**, **C. Wong**, A. Ahmad, B. Ni
- 492 Domino synthesis of 1,2,3,5-tetrasubstituted 1*H*-indoles. **S. Maji**, K. Fobi, E. Ametsetor, R.A. Bunce
- 493 Domino aldol-SNAr-dehydration sequence for [3+3] annulations to prepare quinolin-2(1*H*)-ones and 1,8-naphthyridin-2(1*H*)-ones. **K. Fobi**, E. Ametsetor, R.A. Bunce
- 494 Selective N-functionalization of 1,2,4-triazoles and oxidative cyclization yielding sulfur containing tricyclic heteroarenes. **C. Godfrey**, L. Ardon Munoz, J.L. Bolliger
- 495 Access to substituted tricyclic heteroarenes by an oxidative cyclization reaction. **R. Nakiwala**
- 496 Exploiting visible light triggered formation of *trans*-cyclohexene for the contra-thermodynamic protection of alcohols. **P. Das**
- 497 Probing [3+2] photocycloaddition of oxo-benzocycloheptene (Oxo-BC7) and azides. **O. Alkhamayseh**, S. Kharbanda, G. Eastham, J.D. Weaver
- 498 General photocatalytic activation of alkyl halides: New approaches to recalcitrant substrate. **P. Sharma**
- 499 Catalytic donors and acceptors in electron donor–acceptor complex photochemistry. **N. Shafiei**, T. Tasnim, S. Pitre
- 501 Enantioselective branch-selective hydrogen atom transfer alkene hydrosilylation enabled by potassiumated chiral Lewis base catalyst. **Y. Chang**, J. Jeon
- 502 Biocatalytic aza-Michael addition of aromatic amines to enone using α -amylase in water. **S. Dutt**
- 503 Direct synthesis of α,α -difluoroketones from difluorinated carboxylic acids via acyloxyphosphonium ions. **M. Alam**, S.B. Munoz
- 505 Recent advances in ligand-free palladium-catalyzed reactions using palladium(II) chloride. **J. Pettigrew**, E.S. Eitrheim
- 506 Relay iridium catalyzed C–H bond silylation of anilines. **S. Adhikary**, J. Jeon **Raines**
- 508 Iron carbene initiated cascade reaction to functionalized tetrahydrofurans. **P. Kafle**, I. Sharma
- 509 Copper(II) quinoxalinol complexes for catalytic oxidation of benzylic and heterocyclic alcohols. **X. Huo**, M. Guagliardo, A.E. Gordon
- 510 Cobaloxime-photocatalyzed Minisci reactions under visible light irradiation. **S. Pal**, **S. Pitre**
- 511 Vitamin B₁₂ catalyzed cyclopropanation of olefins. **J.G. Teye-Kau**, S. Pitre, M. Ayodele
- 512 Solid phase approach for activity-based protein profiling in human gut commensal bacteria. **C. Nwike**, A.T. Wright
- 513 Nitrogen editing to access uncharted chemical space in drug discovery. **R. Mukherjee**, B. Ghosh, P. Kafle, R. Welles, I. Sharma
- 514 Linear dichroism and absorption characterization of solution-cast organic semiconductor thin films. **N. Akbar**, M. Furis

- 515** Development of new reagents for the preparation of substituted 1,2,4-triazoles. **A. Norris**, J.L. Bolliger
- 516** Structure-guided design of potent direct-acting antivirals of SARS-CoV-2 and MERS-CoV 3CL proteases. **C. Dampalla**, W. Groutas, K. Chang

Polymer Blends and Composites Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

Cosponsored by PMSE

B.P. Grady, V. Rohatgi, *Organizers*

2:00 - 4:00

- 517** Effects of ball milling on dispersibility of ultra high aspect ratio MWCNTs in polymers by melt mixing. **A. Pappas**, M. Rhue, C. Bavlnka, S. Crossley, B.P. Grady
- 518** Rheological characterization of hydrogels to predict printability for bioprinting. **K. Bartholomew**
- 519** Additive manufacturing and characterization of PLA and wood fiber composites for advanced environmental sustainability. R. Siddique, C. Billings, B. Sherwood, **Y. Liu**
- 520** Matrimid/MOP-18 composite material for high-energy hybrid supercapacitor (HSC) electrodes. **S. Haque**, J.P. Ferraris, K.J. Balkus
- 521** Moisture/hydrophobicity sensing by brightly-phosphorescent nanoparticles constructed by electrostatic/supramolecular complexation of metal complexes into biocompatible polymers. **B. Adeyemi**, S. Farvid, N. MirzaNasiri, M. Omary
- 522** Superior effect of hydrogen peroxide intercalating agent relative to sodium chlorate on thermal conductivity of expanded graphite (EG)/paraffin wax and EG/epoxy composites. **A. Nayal**, S. Danayat, J. Garg
- 523** 3D printability and property optimization for carbon fiber reinforced polymer composites. **X. Liu**, C. Billings, B. Sherwood, Y. Liu

Solar, Fuel, Wind and Future Energy Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

L. Ford, *Organizer*J.L. Liu, J. Titah, W. Wei, *Presiding***2:00 - 4:00**

- 524** Graphene composite materials to enhance photoelectrochemical performance for water splitting. **M.D. Detamo**
- 525** $Ti_4N_3T_x$ MXene as a highly stable universal aqueous energy storage material. **J. Kasten**
- 526** Transition metal oxide/MWCNTs nanocomposites as effective supports for methanol electro-oxidation reaction. **A. Nouralishahi**, M. Nath
- 527** Osage orange (*Maclura pomifera*) derived carbon for high-rate capacitors. **A. Ouellette**, R.K. Gupta
- 528** Exploring the chemistry of hydrogen fuel cells. **A. Rahman**, K. Mody, B. Zhao
- 529** DFT study of cyclohexane-based molecules for hydrogen storage. **E. Sikavitsas**, B. Wang
- 530** Rare earth metal oxide templated-conductive carbon for energy storage application. **A. Umer**, K.J. Balkus
- 156** Lithium-ion batteries separator system modeling. **A.P. Nguyen**

Sustainability and Environmental Issues In Hydrocarbon Production Posters

Omni Oklahoma City Hotel, Oklahoma Station 4-5

B. Bohm, J. Jacob, V. Natalie, *Organizers***2:00 - 4:00**

- 531** Efficient detection and removal of small ring polycyclic aromatic hydrocarbons from water. **H. Fernando**, I. Gautam, N. McDaniel, D. Davis
- 532** Method development and quantification of critically valuable elements in Permian Basin produced waters. **C. Oliver**

Biochemistry

Omni Oklahoma City Hotel, Bricktown

O. Prakash, *Organizer*G. Cook, *Presiding*

- 3:00** Introductory remarks.
- 3:05 533** Directly targeting antibiotic resistance and key virulence factors of ESKAPE pathogens. **C.V. Rice**
- 3:25 534** Albumin nanospheres as a precursor to bifunctional colloids. **B.A. Bartlett**, J. Klier, S. Razavi
- 3:45 535** Flexible heteroarotinoids as potential inhibitors against SARS-CoV-2 proteins. **S. Timsina**, M. Akhter, D.H. Zhou
- 4:05 536** Biochemical analyses of phytochemicals in watercress extracts. **J.R. Villanueva**, A. Fisher, B. Sengupta

- 4:25 537** MetNMR software for metabolite identification and quantification with one- and two-dimensional NMR spectra. **M. Akhter**, S. Timsina, C. Figueroa-Hernández, M. Figueroa-Espinoza, P. Rayas-Duarte, D.H. Zhou

Thursday Special Event Lectures

Special Event Lecture

Omni Oklahoma City Hotel, Oklahoma Station 2

F.D. Blum, M. Rosen, C. Varnado, *Organizers*
M. Rosen, C. Varnado, *Presiding*

4:45 - 5:30

- 721** Vinyl chloride, cancer and technology: How science saved a business. **B. Carroll**

Special Event Lecture

Omni Oklahoma City Hotel, Oklahoma Station 6

F.D. Blum, M. Borunda, *Organizers*
M. Borunda, *Presiding*

4:45 - 5:30

- 722** Diversity in chemistry. **K. Johnson-Winters**

Special Event Lecture

Omni Oklahoma City Hotel, Myriad

F.D. Blum, S. Mohanty, *Organizers*
S. Mohanty, *Presiding*

4:45 - 5:30

- 723** The art of border crossings: Integrative multidisciplinary in the natural sciences.
A. Gronenborn

FRIDAY MORNING, November 17, 2023

Biochemistry

Omni Oklahoma City Hotel, Bricktown

O. Prakash, *Organizer*S. Muthukrishnan, *Presiding*

- 8:00** Introductory remarks.
- 8:05 538** Chitin, a versatile and ubiquitous biopolymer. **S. Muthukrishnan**
- 8:30 539** Conserved STRIPAK complex is required for autophagy in muscle tissue. **Y. Guo**, Q. Zeng, D. Brooks, E. Geisbrecht
- 8:50 540** Development of collagen sponges as a delivery vehicle for branched polythetylenimine (BPEI) in the treatment of chronic wounds. **W. Best**, C.V. Rice
- 9:10 541** Chemically modified DNA aptamers targeting complement Factor B: A promising therapeutic approach for atypical hemolytic uremic syndrome. **H. Duan**, Y. Zhang, B. Geisbrecht
- 9:30 542** Catalytic biofilms for drug metabolite synthesis. **D. Medina**
- 9:50** Break.
- 10:10 543** Activity-based probes for live cell phenotype-dependent microbial selection. **A.T. Wright**
- 10:30 544** Quantification and classification in diabetic retinopathy. **A. Martin**, L. Wilcox, M. Whitekiller, D. Baucom, J. Butcher, C. Valdez
- 10:50 545** Functional difference and its structural basis of *Manduca sexta* pro-moricin-6 and moricin-6. **A. Su**, A. Jha, N. Mishra, T. Kimura, C. Hou, H. Jiang, O. Prakash
- 11:10 546** Development and characterization of branched polyethylenimine (BPEI) resistance in *Staphylococcus aureus*. **C.C. Roedl**, C.V. Rice
- 11:30 547** Getting fuel from maltose (malt sugar). **A. Akram**
- 11:50 548** Biomanufacturing of tumor organoids with heterogenous extracellular matrix for improved drug development. **Y. Kim**, A.D. Avera, J. Park

Biotechnology Innovation and Partnerships

Omni Oklahoma City Hotel, Oklahoma Station 7

C.V. Rice, *Organizer*T. Wavering, *Presiding*

- 8:00 549** Thinking about a startup? Here's where to start.... **T. Wavering**
- 9:15 550** How to fund your startup. **T. Wavering**
- 10:20** Break.
- 10:40 551** How to protect your innovation. **D. Kinsinger**
- 11:45 552** The Amazing Dave: Mentalist/magic show and lunch. **D. Kinsinger**

Community College Chemistry Education: Successes and Strategies

Omni Oklahoma City Hotel, Route 66

T. Pillar-Little, *Organizer, Presiding*

- 8:00 553** Making general chemistry relevant to everyday life. **S.J. Donnelly**
- 8:20 554** Expanding two-year college student learning opportunities by analyzing essential oils with GC-MS. **S.J. Donnelly**
- 8:40 555** Course-based undergraduate research experience for non-major chemistry students at a community college. **M.J. Harvey**
- 9:00 556** Importance of prior knowledge and academic legacy. **D.S. Mason**
- 9:20 557** Preparatory chem program resources developed in the LibreTexts OER that could be of value to community colleges. **R.E. Belford**, L. Poirot, E. Waters
- 9:40 558** Teaching the nature of science to nonmajors through a course-based undergraduate research experience. **M.J. Harvey**
- 10:00** Break/networking.

Materials/Polymer

Omni Oklahoma City Hotel, Oklahoma Station 2

N. Green, R.K. Gupta, *Organizers, Presiding*

- 8:30 559** Quantification of surfactant self-assembled structures in confinement. **A. Striolo**
- 8:50 561** DNA conjugated gold nanorods towards energy transfer complexes. **S. Saleh**, N. Green
- 9:10 562** Universal sorbent for sampling volatile, semi-volatile and reactive compounds for chemical exposure assessments. **E. Kadossov**, M.L. Teicheira, Z.A. Brown, N.F. Materer, A.W. Apblett, S. Shaikh
- 9:30 563** Vacuum regenerative sorbents for humidity and carbon dioxide control in closed loop rebreather systems. **J.R. Tidwell**, E.B. Kadossov, Z.A. Brown, N.F. Materer, A.W. Apblett, M.L. Teicheira, S. Shaikh
- 9:50** Break.
- 10:10 564** Incorporation of ferrocene diols into a polyurethane for increased flame retardancy. C. Yeary, T. Butcher, **C.J. Neef**
- 10:40 565** Polymeric SiCO aerogels for oil-water separation. **H. Hayes**, P. Kroll
- 11:00 566** Curing evolution of acrylate-based UV cross-linkable adhesives. **S. Farsiani**, H. Noori
- 11:20 567** Adsorption of surfactant on colloidal particles. **Z. Abbasian Chaleshtari**, B.P. Grady, J. Harwell
- 11:40 568** Unlocking the power of cations: Synergistic nonionic/anionic surfactant mixtures for enhanced performance. **T. Kobayashi**, K. Kotsi, T. Dong, I. McRobbie, A. Moriarty, P. Angeli, A. Striolo

Organic

Omni Oklahoma City Hotel, Myriad

R.R. Kane, *Organizer, Presiding*

- 8:00 569** Rearrangements of sterically hindered pyridinium salts to access underexplored β -aryl substituted pyridines. A. May, **D. May**, M. McIntosh
- 8:20 570** Non-Minisci radical acylation of substituted pyridines via Breslow-like intermediates. **C.A. Beard**, M. McIntosh
- 8:40 571** Facile condensation of pyridinium ylides: An investigational study with potential applications in synthesis. **T.G. Nolan**, M. McIntosh
- 9:00 572** Metal-free C(sp³)-H functionalization of *o*-picolyl alcohols and amides via radical rearrangement. **J.M. Barrett**, J. Kubik, M. McIntosh
- 9:20 573** Dual role of visible light-activated 1,4-dihydropyridine anions: Alkyl radical precursors and photoreductants in organic transformations. **P. Gallage**, S. Pitre
- 9:40** Break.
- 10:00 574** One-pot formal carboradiofluorination of alkenes: A toolkit for positron emission tomography imaging probe development. M. Rivas, S. Debnath, **S. Giri**, Y. Noffel, X. Sun, V. Gevorgyan
- 10:20 575** Radical perfluoroalkylation reactions mediated by halogen-bonding photocatalysis. **T. Tasnim**, S. Pitre, N. Shafiei
- 10:40 576** Dearomatization reactions of N-methoxy ureas. **N. Parveen**, M.N. Awadalla, C.J. Lovely
- 11:00 577** General approach to photocatalytic activation of unactivated alkyl chlorides. **R. Hanumanthu**
- 11:20 578** Catalyst-free light driven [3+2] cycloaddition. **S. Kharbanda**
- 11:40 579** Selective and functional group tolerance C-H aminoalkylation with photosensitizer and imine. S.K. Ghosh, **L. He**, T. Zilu

Sustainability and Environmental Issues in Hydrocarbon Production

Omni Oklahoma City Hotel, Oklahoma Station 1

Cosponsored by ANYL

V. Natalie, *Organizer*B. Bohm, J. Jacob, *Organizers, Presiding*

- 8:20 580** Speedwise water: Creating a marketplace for produced water commodities using machine learning. **Z. Hildenbrand**
- 8:40 582** Density functional theory of CO₂ and CH₄ interactions with shale surfaces. **L. Tribe**
- 9:00 583** Balloon-based observations of seismic activity. **E. Hough**, Z. Yap, B. Elbing, J. Jacob, S. Krishnamoorthy, D. Bowman
- 9:20 584** Monitoring of carbon dioxide and methane plumes from combined ground-airborne sensors. **J. Jacob**, T. Mitchell, N.F. Materer, T. Ley
- 9:40** Break.

- 10:00 585** Impacts of geochemical rock-fluid interactions on production and carbon storage in Caney Shale of Southern Oklahoma. **G.A. Awejori**, W. Dong, C. Dougty, N. Spycher, F. Xiong, L. Bethel, M. Radonjic
- 10:20 586** Ground Water Protection Council. **D. Yates**
- 10:40 587** Role of a scientific referee in earthquake management. **T. Halihan**
- 11:00 588** Comprehensive geochemical analysis of rock-fluid interactions in Marcellus shale. **L. Bethel Dje**, K.C. Carpenter, G.A. Awejori, F. Xiong, M. Achang, M. Radonjic
- 11:20 589** How clean is clean enough for the beneficial reuse of produced water? **Z. Hildenbrand**
- 11:40 590** Analyzing the environmental impact of a commercial aquaponic system in Taiwan using LCA. **S. Rikitu**

Advances in Catalysis for Organic Synthesis

Omni Oklahoma City Hotel, Oklahoma Station 3

Cosponsored by ORGN

S. Pitre, *Organizer*

D. Romo, *Presiding*

- 8:10** Introductory remarks.
- 8:15 591** Cobalt-catalyzed decarboxylative alkylation reactions. **J.A. Tunge**
- 8:45 592** Amine synthesis by hydrogen-atom transfer and energy-transfer photocatalysis. **R. Comito**, S. Ghosh, L. He, M. Hu, T. Zilu
- 9:15 593** New routes to fused heteroarenes via C–N and C–S bond formation. **J.L. Bolliger**
- 9:45** Break.
- 10:15 594** Predictive process metrics to enable sustainability-driven route selection. **N. Weires**, K. Yamamoto, A. Ortiz
- 10:45 595** s-Block metal-mediated methods and catalysis for organic synthesis. **S. Yruegas**
- 11:15 596** New methods for carbon-hydrogen bond functionalization. **O. Daugulis**

Polymer Blends and Composites

Omni Oklahoma City Hotel, Oklahoma Station 6

Cosponsored by PMSE

B.P. Grady, V. Rohatgi, *Organizers, Presiding*

- 8:10 597** PVAc/GO has a really broad glass transition: It's just hard to observe with DSC. **F.D. Blum**, B. Khatiwada, K. Bastola, R. Vaidyanathan, B.P. Grady
- 8:35 598** Composites from post-consumer polypropylene carpet and HDPE retail bags. **A. Maheshwari**, R. Azarfam, S. Chaudhari, C. Switzer, J. Hanan, R. Vaidyanathan, F.D. Blum, S. Bandla
- 9:00 599** Rapid additive manufacturing of thermosetting resins enabled via radio frequency curing. **E. Harkin**, A. Sarmah, T. Tran, M. Cupich, M. Green
- 9:25** Break.
- 9:45 600** Additive manufacturing and optimization of advanced CNT reinforced nanocomposites through process control of photocurable polymers. **C. Billings**, B. Sherwood, Y. Liu

- 10:10 601** Stable titania nanoparticle silicone encapsulants for high brightness light-emitting diodes. **Y. Ning**, D. Huber
- 10:35 602** Electrically conductive $Ti_3C_2T_z$ MXene-polymer composites from Pickering emulsion polymerization. **H. Cao**, Y. Wang, A. Sarmah, S. Gulati, M. Radovic, J.L. Lutkenhaus, M. Green, E. Pentzer
- 11:00 603** High voltage insulation, fire protection, and gas barrier behavior of polyelectrolyte complex thin films. **J.C. Grunlan**

Undergraduate Poster Session

Omni Oklahoma City Hotel, Oklahoma Station 4-5

T. Smith, *Organizer*

9:00 - 11:00

- 604** Degradation of different priority pollutants using MoO_3 nanoparticles. **N. Araujo da Silva**, R. Lirag
- 605** Advances in the synthesis of anisoucoumaramide. **E. Goldsmith**, **P. Porter**, R.J. Felix
- 606** Computational investigation of Criegee intermediate reactions with carbonyls in the atmosphere. **B.S. Ferris**, A.W. Harrison
- 607** Uncovering design principles for carbon-dioxide-expanded electrolytes. **B.S. Ferris**, E.R. Bartlett, W.H. Thompson
- 608** Using computational chemistry to create pH-specific binding in opioids. **P. Upadhyia**, A.W. Harrison
- 609** Synthesis of a new bipyridinium ligand and exploration toward the formation of macrocyclic molecules with platinum(II). **M.A. Liuzzi Vaamonde**, B.W. Smucker
- 610** Plasma protein binding by two formulations (5% and 10%) of the potential cyanide antidote candidate dimethyl trisulfide (DMTS). **K.C. Black**, **K. Jordan**, D.W. Herath, N.Y. Rafeedie, M.B. Wilson, M.E. Langly, L.J. Rodriguez, K.D. Kelley, L. Kiss, I. Petrikovics
- 611** Thermodynamic computational analysis of the synthesis, structure and characterization of 7-dietilaminocumarin-3-carboxylic acid. **M.T. Espinoza-Nicolas**, C. Maldonado-Dominguez
- 612** Influence of solvent polarity on the extraction of phytochemicals from Watercress leaves: A study using HPLC. **A. Fisher**, J. Villanueva, B. Sengupta
- 613** Impact of ubiquitin on BRCA1/BARD1-UbcH5c (E3-E2) dynamics: A molecular dynamics study. **A. Goldman**, T. Shah, H. Torabifard
- 614** Generation of thin films of biomass burning organic aerosol for measurements of reactive uptake. **J. Barton**, E. Schnitzler, H. Al-Mashala
- 615** Characterizing antibody-tandem repeat binding with capillary and gel electrophoresis. **G. Herrera**, C.R. McEntee, R.J. Whelan
- 616** Engaging perfluoroalkyl bromides as radical precursors using halogen-bonding photocatalysis. **K. Laminack**, T. Tasnim, N. Shafiei, S. Pitre
- 617** Dual photoredox/vitamin B_{12} -photocatalyzed cyclopropanation reactions. **J.J. Lemons**, J.G. Teye-Kau, S. Pitre
- 618** Synthesis of azolines via microwave and ultrasonic radiation. **D. Dao**, E.A. Nalley

- 619 Advancing imidazole research to explore its potential to combat microbial pathogens. **J. Duran Chaves**, E.A. Nalley
- 620 Analysis of BPA leaching from feminine hygiene products using fluorescence spectrophotometry. **M. Rettig**, S.E. Hubbard
- 622 Effect of electron withdrawing periphery groups in pyrrophen UO₂ complexes. **B.D. Hawkins**, J. Ducilon, A.E. Gorden
- 623 Designing an optimal expression system of peptides in *E. coli*. **S. Ramesh**, J.A. Hebda
- 624 Synthesis, characterization, and computational absorption of a germanium palladium complex. **R.C. Newbrand**, M. Leal, B.W. Smucker, A.W. Harrison
- 625 Expression and reactivity of a Baeyer-Villiger monooxygenase from *Thermobifida fusca*. **C. Tebrinke**, M.E. Hinze
- 626 Detection and quantification of lead contamination in ground turmeric. **L.E. Moore**, S.G. Prilliman
- 627 Synthesis of benzimidazoles using planetary ball mill. **L. Hunter**, R. Lirag
- 628 Synthesis and characterization of tridentate quinoline-based NCO ligands. L. Tahsini, N. Noei, **J. Rein**
- 629 Interaction of cisplatin with isolated guanine. **K. Coker**, J. Hernandez, N. Mirsaleh-Kohan, J.D. Beatty
- 630 Temperature-dependent ionic conductivity of a chloride-ion polymer electrolyte. **S. Taylor**, C.M. Burba
- 631 Electrodeposition of ZnO on plastic-based substrates for solar cell applications. **M. Nguyen**, G. LeBlanc
- 632 3D printing and modification of electrodes for use in biosensors. **I. Melton**, G. LeBlanc
- 633 Examining reproducibility and fabrication of thermoresponsive ultrafiltration membranes. **C.M. Pool**, S. Tabatabaei, R. Foudazi
- 634 Intermittent illumination using modern LED technologies to study radical chain reactions. **K. Ashcraft**, M. Ayodele, S. Pitre
- 635 Enantioselective *anti*-aldol reactions of *N, N*-diisopropylphenylacetamides. **J. Davies**, **P.B. Chanda**
- 636 Learning module for a mass flow controller with application in protein studies. **Z. Hall**, A. Newton, A. Perez, D.E. Thompson
- 637 Adjustments to buffer conditions paves way to radiolabel-free RecA strand exchange experiments. **C. Kelley**
- 638 The impact of base redundancy on DNA-binding of *E. coli* RecA. **E. Wirth**
- 639 Platinum-based cancer drugs in US patents and primary chemical literature. **D. Frey**, G. Paniconi
- 640 Exploring the practicality and detection of ChatGPT in General Chemistry I at UCO. E.S. Eitheim, **E. Betchan**, **I. Ramirez**, **G. Mullaney**
- 641 Correlation between air-water interfacial properties and foaming behavior of perfluorooctanoic acid (PFOA). **H.B. McCray**, M. Zhou, R. Foudazi

- 642 Study of iodine distribution and concentrations in western Oklahoma brine waters and recycling of used chloroform. **J.R. Wickham**, J.M. Frame, A. Larson, D. Edlin
- 643 Preparation and analysis of herbal dish detergent. **N. Gaskill**, G. Garusinghe
- 644 Revealing nanoconfinement induced catalytic selectivity at single molecule level. **D. Heffer**, G. Kim, B. Dong
- 645 Addition of phthalimide to styrene oxide using ammonium salts as catalysts. **E. Hammeke**, C.J. Neef
- 646 Examination of cancer cell survival using AI confluence analysis. **A.W. Browning**, J. Pittman, A. Wolfe, H. Rodriguez, O. Zuniga
- 647 Designing a lab: Ascorbic acid method for phosphorus level determination. **M.F. Maltez Navarrete**, C. Beauregard
- 648 Indium(III) triflate, a green catalyst for Friedel-Crafts reactions. **C. Walls**, P. Reeves
- 649 Biosorption of heavy metals in wastewater and utilization of recovered biomass to produce biofuel. **N. Smith**, N. Green, S. Islam, V. Duran, B. Jang
- 650 Optimization of the utilization of photocatalyst chemistry in the Giese reaction. **A. Ethridge**
- 651 Characterization of redbud tree heartwood extracts. **A.E. Rubio**, C. McKinney, N.L. Paiva
- 652 Investigation of methods for quantifying arsenic in water. **H. Strickbine**, **A. DeHoet**, **D. Oberley**, **H. Hua**, **N. Klaus**, A. Oberley
- 653 Structures of a cis- and a trans- isomer of (η^5 -cyclopentadienyl)-carbonyl-(4-chlorophenylthiolato)-iron dimer. L. Holley, **C.D. Bryan**
- 654 Aqueous miscibility of distribution model liquids. **N.E. Nevels**, C. Fennell
- 655 Stability of the Schiff Base of Amino Acid Derived Ni(II) Complexes. **J. Childress**, E. Burgess, B.A. Vinson, A. Jergensen, T.K. Ellis
- 656 Selective N-alkylation of 1,2,4-triazoles and imidazoles. **M. Menefee**, C. Godfrey, J.L. Bolliger
- 657 Reactivity of Ni(II) complexes of glycine toward alkylation under kinetic reaction conditions. **A. Jergensen**, J. Le, T.K. Ellis
- 658 Quantifying ideality in liquid mixtures with quadratic curvature analysis. **C. Severin**
- 659 Determination of pKa's in glycine-metal complexes under aprotic solvent conditions. **J. Garcia**, A. Crisp, T.K. Ellis, J. Henrikson
- 660 Design and synthesis of *Double-ESIPT* fluorescent probes for multi-analytes detection. R. Mia, **B. Maillet**
- 661 Intersection of XPO7 and TP53 pathways in breast cancer. **M. Duut**, A. Olschefski, M. Joshi
- 662 Computational method in modeling piezoelectrically-induced quantum wells. **L. Vilshansky**, M.B. Santos, K. Mullen
- 663 Catalytic photoredox dimerization of active methylene compounds. **J. Sangalli**, A. Acharya, R. Giri
- 664 Identification of impurities in EuScO₃ crystals using electron paramagnetic resonance. **S. Martin**, A. Pambukhchyan, M. Coumans, E. Haliman, L. Bouchard, S. Takahashi

- 665 *Anti*-selective enolboration-aldolization of *N, N*-dialkylarylamides. **D.J. Schwaibold, P.B. Chanda**
- 666 Light absorbance of biomass burning organic aerosol from eastern red cedar in methanol and water. **H. Anthony**, C. Calvert, H. Al-Mashala, K.L. Betz, E. Schnitzler
- 667 Competitive vs. synergistic surfactant adsorption. **D.S. Barrios Perez**
- 322 Synthesis of substrates and standards to investigate biocatalytic chiral resolutions through oxidation. **S.M. Simmons**
- 361 Synthesis and characterization of bis-urea organogelators with a two-carbon spacer. **S. Kaul, A.J. Carr**
- 364 Synthesis and characterization of bis-urea organogelators with a three carbon spacer. **V. Melchor, A.J. Carr**

FRIDAY AFTERNOON, November 17, 2023

Advances in Catalysis for Organic Synthesis

Omni Oklahoma City Hotel, Oklahoma Station 3

Cosponsored by ORGN

S. Pitre, *Organizer*D. Romo, *Presiding*

- 1:00 668** Revisiting DMAP catalyzed acylations of alcohols: ^{13}C kinetic isotope effects, and same excess protocols explore pre-equilibrium. **E. Plata**, T.V. Alvarez Carmona, S. Ortega, A. Mar, F. Cisneros, B. Sosa, I. Al-Qudah, S. Peña, M. Cooke, G. Alvarez, A. Perez, S. Guerra, M. Kim, D. Hayes, R. Spinks, P. Zepeda, F. Hernandez, H. Morales
- 1:30 669** Traceless activation strategies for nitrene transfer chemistry. **D. Powers**
- 2:00 670** Impurity synthesis in support of purge factor analysis in commercial manufacturing. **S. Sundstrom**, M.C. Hillier, C. Yang
- 2:30** Break.
- 3:00 671** Acyloxyphosphonium ions derived from (fluoro)carboxylic acids feedstocks as versatile building blocks for diverse catalytic transformations. **S.B. Munoz**
- 3:30 672** New strategies in copper-catalyzed oxidative decarboxylation reactions. **J.M. Hoover**
- 4:00 673** New cross-coupling reactions to access natural product space and interrogate its biology. **R.A. Shenvi**

Biotechnology Innovation and Partnerships

Omni Oklahoma City Hotel, Oklahoma Station 7

C.V. Rice, *Organizer*T. Wavering, *Presiding*

- 1:00 674** Startup founders panel. **T. Wavering**
- 2:05** Break.
- 2:25 675** Design thinking workshop – bring innovation to your research. **C. Rigsby**
- 3:30 676** Networking mixer. **C.V. Rice**

Evidence Based Pedagogies and General Papers in General Chemistry

Omni Oklahoma City Hotel, Bricktown

J. Mutambuki, *Organizer, Presiding*C.Z. Muteti, *Presiding*

- 1:00** Introductory remarks.
- 1:05 677** Teaching organic chemistry with drag and drop questions and control experiments. **R. Comito**
- 1:25 678** Metacognition instruction relinquishes the existing equity gaps in study strategies across student demographic groups in general chemistry I course. **C.Z. Muteti**, B. Jacob, J. Mutambuki

- 1:45 679** Voices of STEM role models versus metacognition training: How do they impact students' perceptions of chemistry and science? **S. Puvanendran**, T. Kerr, C.Z. Muteti, J. Mutambuki
- 2:05 680** Making them see the relevance: The impact of incorporating real-world contexts on students' perceptions of the content and performance in General Chemistry-I lecture course. **I. Sristy**, Y. Vasquez, J. Mutambuki
- 2:25 681** Integrating relevance in the general chemistry laboratory investigations increases students' mastery of concepts and development of scientific skills. **J. Mutambuki**, F. Awudu
- 2:45** Break.
- 3:05 682** Price of precision: Significant figures and cognitive load. **R. Britt**, M. Weinrich
- 3:25 683** Development of a set of best practices for particulate representations in introductory chemistry. **S.G. Prilliman**
- 3:45 684** Peer review as a tool for supporting science practice engagement. **A.C. Moon**
- 4:05** Concluding remarks.

Generative AI: A Game-Changer for the Future of Learning and Research

Omni Oklahoma City Hotel, Route 66

M.J. Czapla, E.S. Eitrhein, *Organizers, Presiding*

- 1:00 686** Navigating the ethical dilemmas of generative A.I. in chemistry learning. **E.S. Eitrhein**
- 1:20 687** Intelligent design and optimization of high-performance synthetic polymers through AI-driven machine learning. **M. Gudavalli**, S. Narisetty
- 1:40 688** Using AI to stimulate critical thinking in community college classes. **F.K. Wood-Black**
- 2:00 689** Artificial intelligence as a teaching assistant for chemistry classes. **L. Bello**
- 2:20 690** Cyberlearning: AI as expert systems in organic chemistry teaching. **D.J. Nelson**
- 2:40** Break.

Organic

Omni Oklahoma City Hotel, Myriad

R.R. Kane, *Organizer, Presiding*

- 1:00 691** Expanding applications of oxidative biocatalysts for synthesis. **M.E. Hinze**
- 1:25 692** Unlocking the potential of nitrous oxide as a chemical feedstock – modeling and developing reactions of N₂O with nucleophiles. **K.M. Nicholas**, I. Sharma
- 1:50 693** Metal carbenes for stereoselective glycosylation. **S. Singh**, B. Ghosh, I. Sharma
- 2:15 694** Thermal rearrangements of dialkynylazoles. **S.M. Kerwin**
- 2:40 695** Application of Ni(II) complexed Schiff bases for the preparation of α-amino acids. **T.K. Ellis**
- 3:05** Break.

- 3:25 696** Development of new oxysterol-binding protein (OSBP)-targeting antiviral and anticancer compounds. **J.L. Berrios-Rivera**, S. Nimmo, R. Bui, R. Bayimenye, S. Choudhary, A.W. Burgett
- 3:45 697** Studies toward a total synthesis of dimeric pyrrole-imidazole alkaloids – ageliferin. **N. Dey**, M. SinghaRoy, C.J. Lovely
- 4:05 698** Development of a concise asymmetric total synthesis of ceratinadin B: Construction of the imidazolyl-quinolone framework. **A. Ghorai**, X. Meng, C.J. Lovely
- 4:25 699** Exploring new inhibitors for SARS-CoV-2 main protease. **S.H. Abdelwahed**

Undergraduate Research

Omni Oklahoma City Hotel, Oklahoma Station 6

T. Smith, *Organizer*

E.A. Nalley, D.J. Nelson, *Presiding*

- 1:00 700** TDA/TD-DFT benchmark for the excited states of secondary photosynthetic pigments. **E. Contreras Cuevas**, G. Mondragón-Solórzano, J. Barroso-Flores
- 1:15 701** New osmium carbonyl complexes with NCN-type ligands. **A.H. Schumacher**, C.B. Powell, G.L. Powell
- 1:30 702** Preparation of osmium complexes for aptamer-based sensors. **E.E. Osborn**, A.H. Schumacher, C.B. Powell, G.L. Powell
- 1:45 703** Comprehensive study of specific enthalpy of different simple carbohydrates and aromatic hydrocarbons. **K. Kervin**, S. Pratihar
- 2:00 704** Synthesis and spectroscopic analysis of a germanium molybdenum complex. **A. Welch**, M. Leal, A.W. Harrison, B.W. Smucker
- 2:15 705** High temperature reactions of osmium carbonyl with 3-*tert*-butylpyrazole and indazole. **N.P. McKinney**, **N.J. Palomino**, C.B. Powell, **G.L. Powell**
- 2:30 706** Synthesis, characterization, and computational absorption of a germanium-platinum complex. **C.A. Suarez**, M. Leal, B.W. Smucker, A.W. Harrison
- 2:45 707** The use of CRISPR knock-ins to generate a triple reporter cell line. **F. Goodavish**, S. Bahraoui, L. Banazysnki
- 3:00 708** Effect of surfactant-polymer complexation in precursor on final hydrogel properties. **S. Onyembe**, M. Zhou, R. Foudazi
- 3:15** Break.
- 3:30 709** Synthesizing a catenulobactin B analog: Paving the path to novel sideromycins. **A. Whitner**, V. Greer, T. Quarcoopome, P.K. Desman
- 3:45 710** Developing humanized PNPLA3 mice. **K. Dempsey**, Y. Wang, G. Liang, J. Cohen, H. Hobbs
- 4:00 711** Thermoresponsive membranes from lyotropic liquid crystal templates. **A. Headley**, Y. Saadat, R. Foudazi
- 4:15 712** Designing catalyst-free, strain-loadable alkenes as photo click reagents for biological uses. **G. Eastham**, S. Kharbanda, O. Alkhamayseh, J.D. Weaver

- 4:30 713** Nickel coated 3D printed electrodes for electrochemical applications. **B.D. Charles**, H. Dang, G. LeBlanc
- 4:45 714** Electrodeposition of perovskite solar cell materials. **E. Falconetti**, G. LeBlanc
- 5:00 715** Determination of ascorbic acid content within store-bought kombucha using UV-spectrophotometry and multivariate regression modeling. **C. Williams**, J.R. Ingle