SWRM #80

2024 Southwest Regional Meeting

of the

American Chemical Society

Waco, Texas

October 20-23, 2024

K. L. Shuford, *Program Chair*

R.R. Kane, *General Chair*

MEETING AT A GLANCE

Sunday 10/20

7 am – 6 pm	On-site registration	WCC Event Office (upper atrium)
7 – 8 am	Senior Chemist's Breakfast	Hilton Brazos Grill
8 am – 12 pm	Technical Program	WCC Lower Level (various rooms)
10 -10:30 am	Coffee Break	WCC Upper Atrium
1 – 5 pm	Technical Program	WCC Lower Level (various rooms)
3 -3:30 pm	Coffee Break	WCC Upper Atrium
5 – 5:45 pm	Dial-Black Reception	Hilton Three Rivers Ballroom
5:45 - 7 pm	Dial-Black Lecture (Paul Wender)	WCC McLennan Hall (upper level)
7 – 9 pm	Welcome Reception/Poster Session 1	WCC Brazos Ballroom (upper level)
7 – 9 pm	EXPO & Grad Fair	WCC Brazos Ballroom (upper level)

Monday 10/21

7 am – 6 pm	On-site registration	WCC Event Office (upper atrium)
7 – 8 am	Senior Chemist's Breakfast	Hilton Brazos Grill
7:30 – 9 am	Refreshments at Baylor Networking Hub	WCC Upper Atrium
8 am – 12 pm	Technical Program	WCC Lower Level (various rooms)
10 -10:30 am	Coffee Break (sponsored by ACS Marketing)	WCC Brazos Ballroom (upper level)
10 am – 1 pm	EXPO	WCC Brazos Ballroom (upper level)
12 – 1:30 pm	High School Educators Lunch	Ranger 108 (WCC Lower Level)
12 – 1:30 pm	Undergraduate lunch/awards/grad panel	Chisolm Hall (WCC Lower Level)
1 – 5 pm	Technical Program	WCC Lower Level (various rooms)
3 -3:30 pm	Coffee Break (sponsored by Merck)	WCC Brazos Ballroom (upper level)
4:30 – 6 pm	Undergrad social/Ask a chemist!	Chisolm Hall (WCC Lower Level)
4:30 – 6 pm	WCC Coffee (sponsored by ACS/PROF/WCC)	Ranger 108 (WCC Lower Level)
5 – 5:45 pm	Gooch-Stephens Reception	Hilton Three Rivers Ballroom
5:45 - 7 pm	Gooch-Stephens Lecture (Mark Johnson)	WCC McLennan Hall (upper level)
7 – 9 pm	Gala Reception/Poster Session 2	WCC Brazos Ballroom (upper level)
7 – 9 pm	EXPO & Grad Fair	WCC Brazos Ballroom (upper level)

Tuesday 10/22

7 am – 5 pm	On-site registration	WCC Event Office (upper atrium)
7 – 8 am	Senior Chemist's Breakfast	Hilton Brazos Grill
7:30 – 9 am	Merck recruiting breakfast (students and postdocs)	WCC Chisolm Hall (lower level)
8 am – 12 pm	Technical Program	WCC Lower Level (various rooms)
10 -10:30 am	Coffee Break (sponsored by Bruker)	WCC Brazos Ballroom (upper level)
10 am – 1 pm	EXPO	WCC Brazos Ballroom (upper level)
1 – 5 pm	Technical Program	WCC Lower Level (various rooms)
3 -3:30 pm	Coffee Break	WCC Brazos Ballroom (upper level)
3 – 4 pm	ACS Governance Reception	WCC Brazos Ballroom (upper level)
3 – 5 pm	EXPO	WCC Brazos Ballroom (upper level)
5:45 - 7 pm	Gooch-Stephens Lecture (Andrew Ellington)	WCC McLennan Hall (upper level)
7 – 9 pm	Poster Session 3	WCC Brazos Ballroom (upper level)

Wednesday 10/23

7 am – noon	On-site registration	WCC Event Office (upper atrium)
7:30 – 11:30 am	Southwest Region Board Meeting	WCC Waco Room (lower level)
8 am – 12 pm	Technical Program	WCC Lower Level (various rooms)
10 -10:30 am	Coffee Break	WCC Upper Atrium
12 – 1:30 pm	Awards Luncheon (ticketed)	Hilton Brazos Room
1 – 5 pm	Technical Program	WCC Lower Level (various rooms)
3 -3:30 pm	Coffee Break	WCC Brazos Ballroom (upper level)

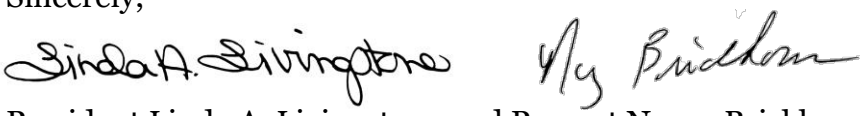
Baylor University

Welcome to Waco, Texas and the 2024 Southwest Regional Meeting of the American Chemical Society! Baylor University's Department of Chemistry and the local Heart of Texas section of ACS are proud to serve as this year's hosts. We share your commitment to meaningful research, experiential learning opportunities for students, and continuing education for professionals.

Baylor University is grateful to Dr. Kevin Shuford, Dr. Bob Kane, and the entire conference planning committee for putting together this robust conference schedule. We hope you enjoy your time meeting with and learning from fellow chemists, especially your plenary speakers, Dr. Paul Wender, Dr. Mark Johnson, and Dr. Andrew Ellington. We also hope that while you are here, you take time to visit Baylor's beautiful campus and enjoy all our city has to offer.

We are excited you are here, and wish you a wonderful SWRM 2024!

Sincerely,



President Linda A. Livingstone and Provost Nancy Brickhouse

American Chemical Society

1155 SIXTEENTH STREET, N.W.
WASHINGTON, D.C. 20036
Phone 202-872-4461
president@acs.org

OFFICE OF THE PRESIDENT

Mary K. Carroll, Ph.D.
President-Elect, 2023
President, 2024
Immediate Past President, 2025

September 23, 2024

Dear Southwest Regional Meeting Participants:

On behalf of the more than 200,000 individuals in the American Chemical Society's global community, I am delighted to extend my warm personal greetings to all of you attending the ACS Southwest Regional Meeting (SWRM) in Waco, TX.

The three plenary lectures include the Dial-Black Lecture presented by Paul Wender of Stanford University on Sunday evening, and lectures by the Gooch-Stephens awardees who will each deliver a technical talk and general lecture: Mark Johnson of Yale University (Monday morning technical talk; Monday evening general lecture) and Andrew Ellington of the University of Texas at Austin (Tuesday evening general lecture; Wednesday morning technical talk).

Please take advantage of the numerous symposia including over 840 presentations spanning dozens of subspecialties including metalloenzyme design, materials for energy and the environment, chemical reaction kinetics, dynamics, and mechanisms, DNA damage detection, tolerance, and toxicity, and targeting the tumor microenvironment, among many others. There will also be sessions highlighting undergraduate research, a high-school educators symposium, and ACS career and technical workshops. There are also many special opportunities for high school teachers and undergraduates, and events sponsored by industrial partners and ACS committees.

I encourage everyone to attend the expo, the coffee breaks (10 AM and 3 PM daily), the Dial-Black and Gooch-Stephens receptions, as well as the Award Symposium on Wednesday, October 23 at noon, honoring the recipients of the Southwest Region ACS Award, the E. Ann Nalley Regional Award For Volunteer Service, the Stanley C. Israel Regional Award, the Partners for Progress and Prosperity (P3) Award, and the Regional Award For Excellence In High School Teaching.

For all these great symposia, workshops, and various social events, I want to express my special thanks to the SWRM General Chair Bob Kane, Program Chair Kevin Shuford, Biological Chemistry Chair Michael Trakselis, Awards Chair Amy Millsap, Expo Chair Touradj Solouki, the many organizers, volunteers, ACS staff, and especially our hosts from the Heart o' Texas Section for their hard work and dedication to create an intellectually stimulating, diverse, and inclusive experience here in Waco.

Best wishes for a most successful 2024 SWRM!

Mary K. Carroll
President
American Chemical Society

Waco Convention Center Info

WiFi - complimentary WiFi will be available in the Convention Center during the meeting.

WiFi Network Name: ccpublic
Password: wacocc17

Beverage Services - water stations will be available outside the meeting rooms. Complimentary coffee and tea and other beverages will be available daily from 8 am - 5 pm in the WCC upper atrium.

Networking Space - Networking space sponsored by Baylor University can be found in the WCC upper atrium.

FOOD and Drink - There is an abundance of convenient locations for great meals. The following are in/adjacent to the WCC:

In the Convention Center

Upper Atrium
Daily 11 am - 2 pm
Sunday 5 pm - 8 pm

Brown Bag Special

Pulled Pork Sandwiches
Brisket Sandwiches
Sausage Sandwiches
Chips
Sodas/water
BBQ Frito pie
BBQ Nachos

EST. 2020
HILLARD
BARBECUE

Located Upstairs
Kiosk

In the Hilton

Breakfast, lunch, and dinner daily

Brazos Grille

Brazos Grille at the Hilton Waco hotel offers a variety of regional Italian inspired dishes to meet everyone's tastes at an affordable price. Offering a casual, yet festive atmosphere with a wide variety of menu selections, it provides the perfect place to enjoy the panoramic views of Indian Hills Park & the Brazos River. Brazos Grille is open daily for breakfast, lunch and dinner serving fresh indigenous local products.

Across the Street

BANGKOK ROYAL
Authentic Thai Cuisine

Ninfa's
Mexican Restaurant

Teriyaki Park

DIAMONDBACK'S
A TEXAS STEAKHOUSE

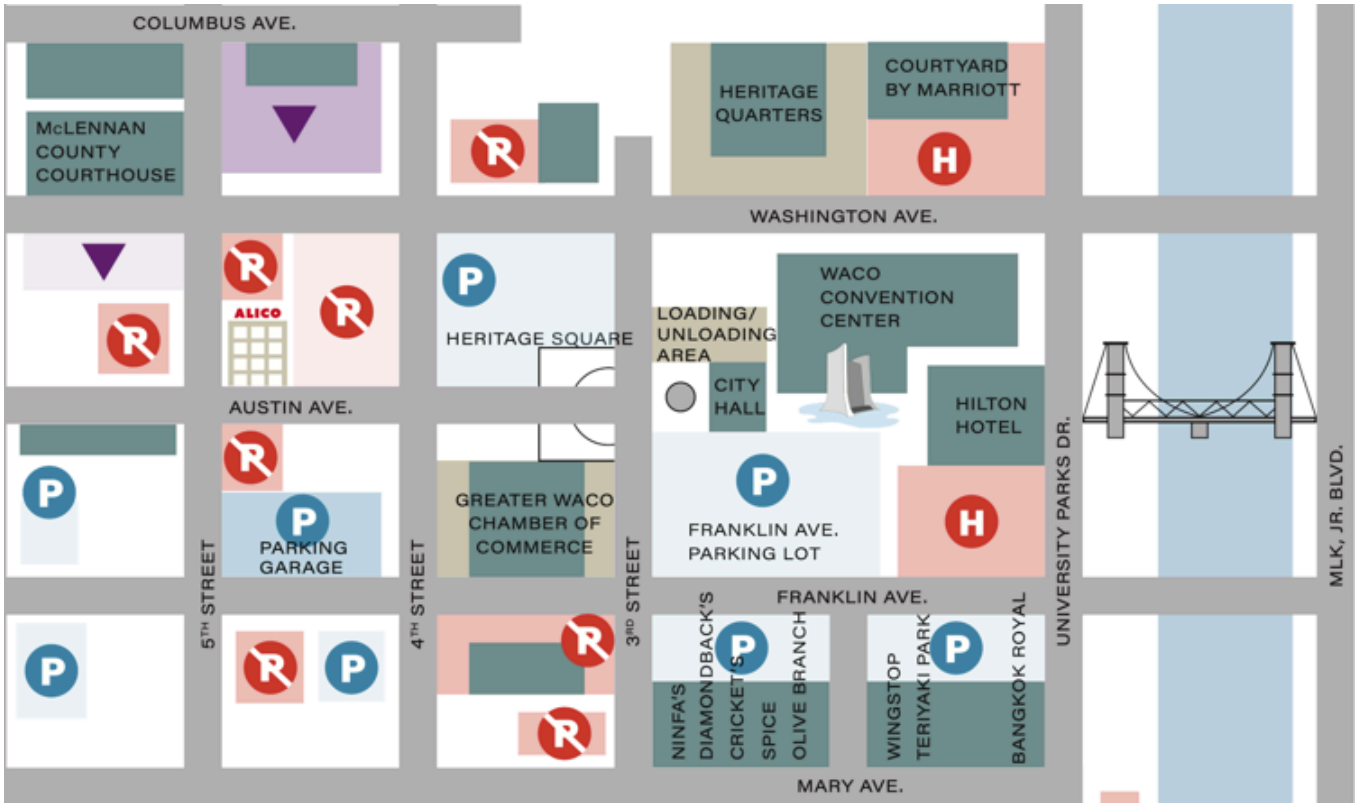
CRICKET'S
DRAFT HOUSE + GRILL

Original Bitty & Beau's Coffee Est 2016

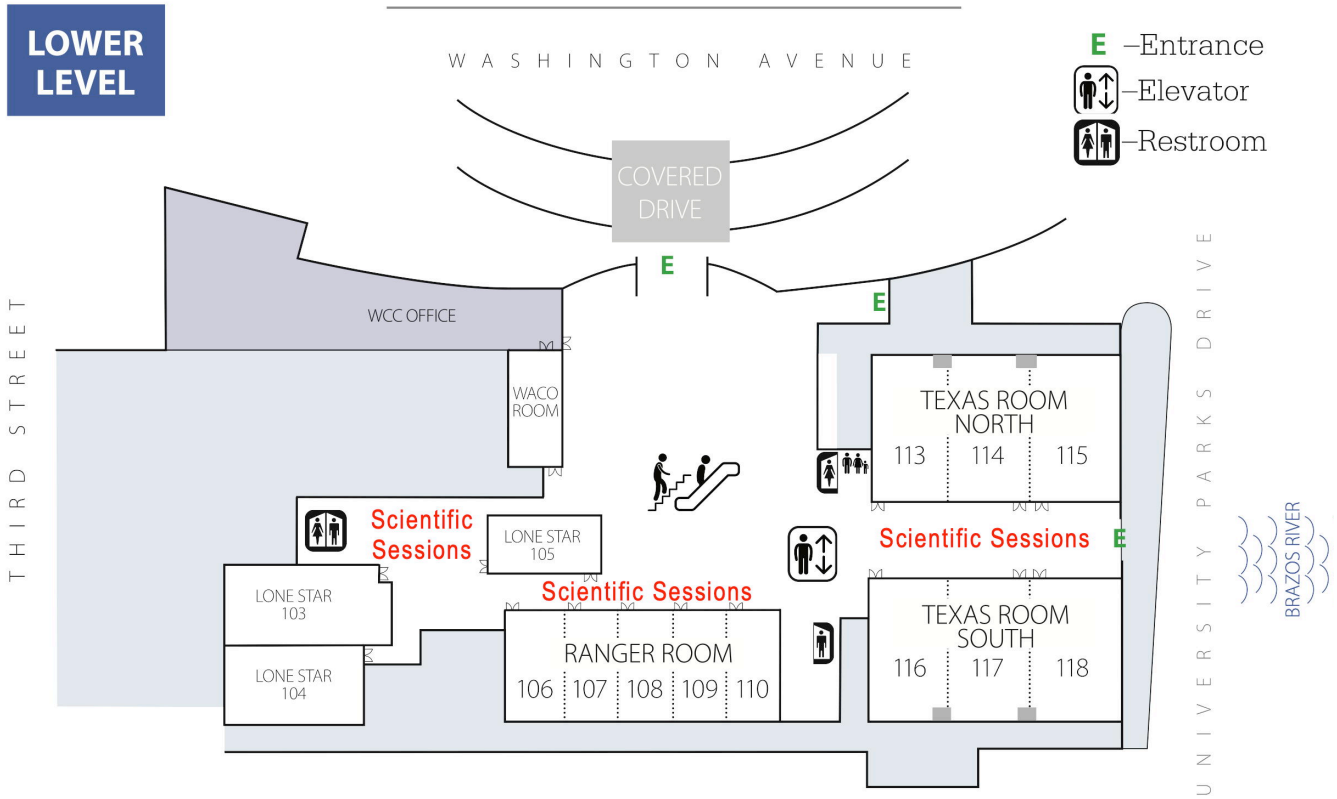
the Olive Branch
Bistro • Bakery

Meeting Location – Meeting activities will be in the Waco Convention Center (WCC), located at 100 Washington Avenue, Waco 76701. Registration will be on the second level at the Event Office beginning at 7 am Sunday morning.

Parking – there are over 900 free parking spots adjacent to the Convention Center and in lots surrounding the Convention Center (see below). Especially convenient are the Franklin Ave and Heritage Square lots right next to the Convention center and the Franklin Avenue parking garage. All are free! A map can be found at https://wacocc.com/wp-content/uploads/2024/04/Waco-Downtown-Parking-Map-4-11-2024.pdf



LOWER LEVEL



A virtual tour of the Waco Convention Center is available at WacoCC.com.

UPPER LEVEL

Refreshments??

SWRM 2024 has you covered - Beverages will be available ALL DAY LONG!

9:30 am - 2 pm

Coffee (regular and decaf), hot herbal teas, and water

2 pm - 5 pm

Coffee (regular and decaf), lemonade, and water

WHERE??

Sunday - Upper Atrium, WCC

Monday - Brazos Ballroom, WCC

Tuesday - Brazos Ballroom, WCC

Wednesday - Upper Atrium, WCC

Scheduled Coffee Breaks

Sunday 10-10:30 am; 3-3:30 pm

Monday 10-10:30 am (Sponsored by ACS)

Monday 3-3:30 pm (Sponsored by Merck)

Tuesday 10-10:30 am (Sponsored by Bruker)

Tuesday 3-3:30 pm

Wednesday 10-10:30 am; 3-3:30 pm

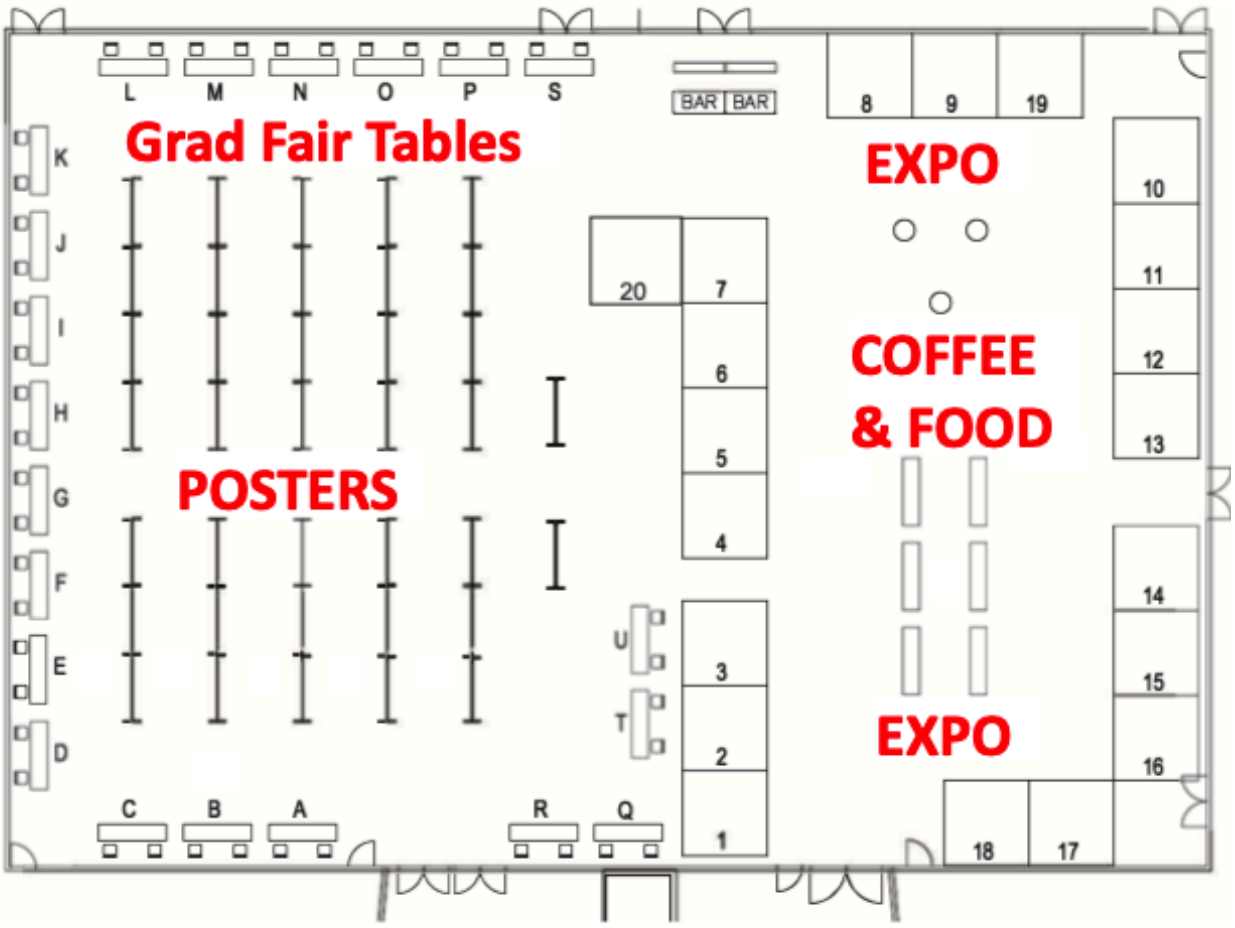
EXPO

Sunday 10/20 7-9pm
Monday 10/21 10am-1pm; 7-9pm
Tuesday 10/22 10am-1pm; 3-5pm

The SWRM EXPO will be in the WCC Brazos Ballroom

WCC Brazos Ballroom Floorplan

(Upper Level)



Grad Recruiting Tables

A	Texas Tech University	L	OU Bioprocessing
B	Rice University	M	Texas Woman's Univ
C	UT Arlington	N	University of Arkansas
D	Texas A&M University	O	UT El Paso
E	Baylor Chem&Biochem	P	Sam Houston State U
F	Baylor Env. Science	Q	University of Memphis
G	UT Dallas	R	Louisiana State U
H	U Michigan Med	S	Oklahoma State U
I	Baylor College of Med	T	Baylor Material Sci Eng
J	New Mexico State U	U	UT San Antonio
K	University of Oklahoma		

EXPO Booths

1	Chem21Labs	11	Cytiva
2	Nanalysis	12	Buchi
3	JEOL	13	Oakwood
4	Advion	14	GEA
5	Bruker	15	Vici
6	Edwards Vacuum	16	ChemGlass
7	Schimadzu	17	ACS
8	Millipore Sigma	18	Agilent
9	Merck	19	ATS Sci. Products
10	ThermoFisher	20	Waters

Undergraduate Oral Presentations

Ranger 106-107 (WCC Lower Level)
Sunday 10/20 1 - 5 pm
Monday 10/21 8 am - 12 pm

Undergraduate Poster Presentations

Brazos Ballroom (WCC Upper Level)
Sunday 10/20 7 - 9 pm

Undergraduate Luncheon/Awards/Grad Panel

Chisolm Hall (WCC Lower Level)
Monday 10/21 12 - 1:30 pm

Undergraduate Social/Ask-a-scientist

Chisolm Hall (WCC Lower Level)
Monday 10/21 4:30 - 6 pm

Graduate Recruiting Fair

Brazos Ballroom (WCC Upper Level)
Sunday 10/20 7 - 9 pm
Monday 10/21 7 - 9 pm

Baylor Sciences Building Tour/Lunch

Sign up at Baylor Chem & Biochem recruiting table
Meet at WCC front entrance (Washington St.)
Tuesday 10/22 11 am - 1 pm

2024 AWARDEES

SOUTHWEST REGION ACS AWARD

Virender K. Sharma
Professor and Director of the Program on Environment and Sustainability
Texas A&M University

The Southwest Region ACS Award recognizes a person who, during a period of residence in the Southwest Region of the ACS, has made meritorious contributions to the advancement of chemistry, chemical engineering, chemical education, either pure or applied, to the profession in general.

E. ANN NALLEY REGIONAL AWARD FOR VOLUNTEER SERVICE

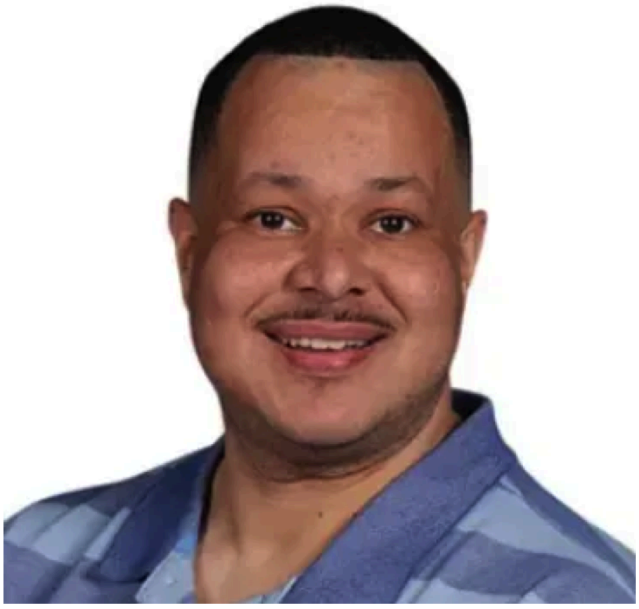
John O'Brien
Dow Chemical

The Ann Nalley Regional Award for Volunteer Service to the American Chemical Society was instituted in 2006 by ACS Past President E. Ann Nalley as part of her presidential initiative to recognize ACS volunteerism.

STANLEY C. ISRAEL REGIONAL AWARD

Rafael Verduzco
Professor and Associate Chair, Chemical & Biomolecular Engineering
Professor, Materials Science & Nanoengineering
Rice University

The Stanley C. Israel Regional Award for Advancing Diversity in the Chemical Sciences recognizes individuals and/or institutions that have advanced diversity in the chemical sciences and significantly stimulated or fostered activities that promote inclusiveness within the ACS Regions.



SOUTHWEST REGION AWARD FOR EXCELLENCE IN HIGH SCHOOL TEACHING

Antoine Lorenzo Foster
St. Michael the Archangel High School
Baton Rouge, Louisiana

The Division of Chemical Education (DivCHED) established an endowment to support **Regional Awards for Excellence in High School Teaching** in each of the ACS Regions.

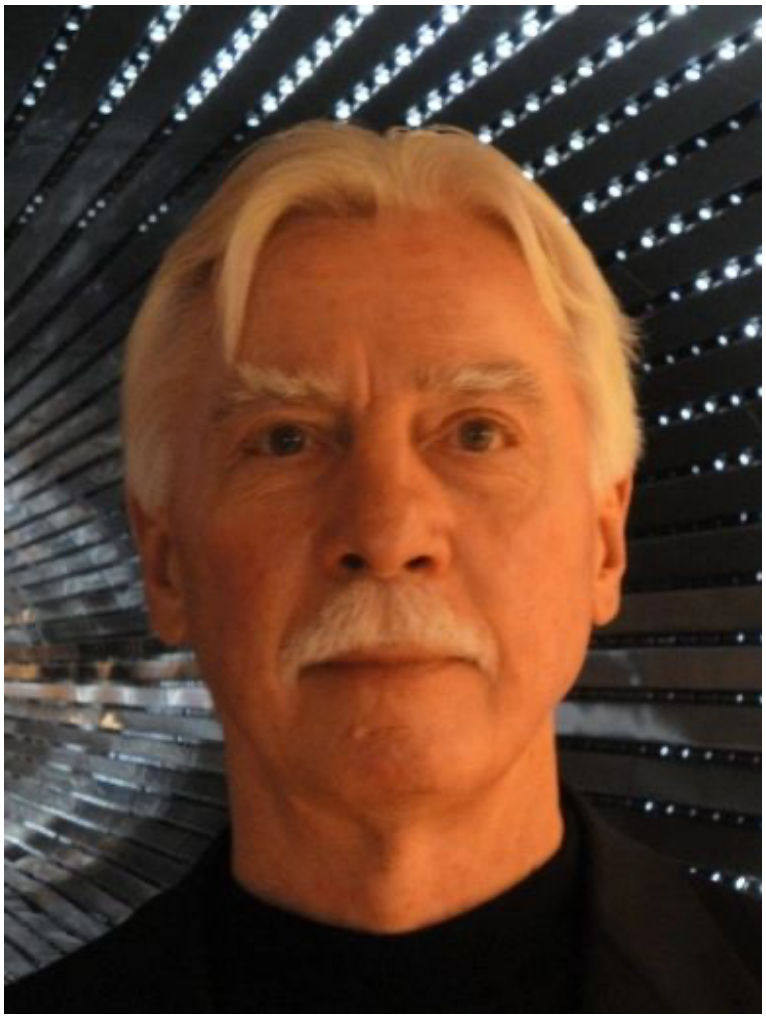
PARTNERS FOR PROGRESS AND PROSPERITY (P3)

https://www.createatx.org/
Sean Roberts and Emily Que
University of Texas
Shawn Amorde , Samanth Soebbing, and Purna Murthy
Austin Community College

The Partners in Progress & Prosperity (P3) Award celebrates successful partnerships between two (or more) organizations with a presence in the Southwestern Region (industry, academia, government, small business, and other domestic or overseas entities, e.g., local sections, international ACS chapters, ACS divisions, other chemical or other professional societies) that have had an impactful outcome, within the Southwestern Region, in one of the following categories: Improving the public perception and appreciation for chemistry Promoting career advancement opportunities and/or supporting entrepreneurship in the chemistry enterprise Advancing advocacy efforts with government and/or other thought leaders Supporting STEM education and/or research

The 2024 SWRM PLENARY LECTURES

W. DIAL BLACK HONOREE



Professor Paul Wender
Bergstrom Professor of Chemistry

Department of Chemistry
Stanford University

"Translational Science: The Chemistry-Biology-Medicine Continuum"

5:45 pm Sunday, October 20
McLennan Hall, Waco Convention Center

Reception 5pm

Hilton 3-Rivers Ballroom
The W. Dial Black Family Lecture
Professor Paul Wender
"TRANSLATIONAL SCIENCE: THE CHEMISTRY-BIOLOGY-MEDICINE CONTINUUM"
Sunday, October 20, 2024
McLennan Hall, Waco Convention Center

The W. Dial Black Lecture is part of an annual lecture series in honor of Sadie Jo Black in the Department of Chemistry and Biochemistry at Baylor University. The Department is pleased to announce that Professor Paul Wender will present the 2024 W. Dial-Black Family Lecture.

Paul Wender received his B.S. degree from Wilkes University and his Ph.D. in chemistry from Yale University. He was an NIH Postdoctoral Fellow at Columbia University. He served on the faculty at Harvard University and joined the faculty at Stanford University where he is the Francis W. Bergstrom Professor of Chemistry and holds a courtesy appointment in the Department of Chemical and Systems Biology. Professor Wender's research has been recognized with numerous awards including recently the Tetrahedron Prize, Prelog Medal (Swiss Federal Institute of Technology), Arthur Cope Award (American Chemical Society), Cohen Award for Excellence in Medicinal Chemistry (Israel Chemical Society), and Research Award of the German Bioactives and Biotechnology Leibniz Allaince. He has also been recognized with several teaching awards including the Hoagland Prize, Bing Teaching Award, and the Dean's Teaching Award. He is an elected member of the US National Academy of Sciences, a foreign member of the Royal Spanish Academy of Sciences, and a fellow of the American Association for the Advancement of Science and the American Academy of Arts and Sciences.

About the W. Dial Black family lecture series
Sadie Jo Black graduated from Baylor University in 1950 and was an assistant professor at Baylor in the Family and Consumer Sciences Department, retiring in 1992 after completing 35 years of service at the university. Growing up in Teague, Texas, her parents, Dial and Tula Black, instilled in her and her brother, William Dial "Dub," the love of God and His church and peoples, as well as the responsibility of sharing. When she learned about promising cancer research being conducted at Baylor, she was committed to enhancing these efforts, and established an endowment that provides funding for a distinguished lecturer series focusing on preeminent research in cancer, Parkinson's disease, or other major diseases. The W. Dial Black Family Lectures bring multidisciplinary speakers in chemistry, molecular biology, and other suitable fields of interest to Baylor University.

The 2024 SWRM PLENARY LECTURES

GOOCH-STEPHENS HONOREE - MONDAY

Professor Mark Johnson
Arthur T. Kemp Professor of Chemistry

Department of Chemistry
Yale University

"Capturing the molecular level mechanics driving bulk chemical behaviors from catalysis to the spectral dynamics of interfacial water with cryogenic ion spectroscopy"

5:45 pm Monday October 21
McLennan Hall, Waco Convention Center

Reception 5pm
Hilton 3-Rivers Ballroom

Professor Mark Johnson
Technical Lecture in "Chemical Reaction Kinetics, Dynamics, and Mechanisms" Symposium
TEMPERATURE- AND SIZE-DEPENDENT, WATER-CLUSTER-MEDIATED LONG RANGE PROTON TRANSFER IN MICROHYDRATED 4-AMINOBENZOIC ACID

Monday, October 20, 2024. 11:30 AM
Lonestar 103, Waco Convention Center

Award Lecture
CAPTURING THE MOLECULAR LEVEL MECHANICS DRIVING BULK CHEMICAL BEHAVIORS FROM CATALYSIS TO THE SPECTRAL DYNAMICS OF INTERFACIAL WATER WITH CRYOGENIC ION SPECTROSCOPY
5:45-7 pm Monday October 21, 2024
McLennan Hall, Waco Convention Center

The Gooch-Stephens Lectures are an annual event of the Department of Chemistry & Biochemistry at Baylor University, and honor two former Chairs of the Department – Dr. W.T. Gooch and Dr. W.R. Stephens. The Department is pleased to announce that Dr. Mark Johnson is one of two 2024 Gooch-Stephens Lecturers.

Mark Johnson is the Arthur T. Kemp Professor in the Department of Chemistry at Yale University. Johnson is known for the development and exploitation of experimental methods that capture and structurally characterize transient chemical species, such as reaction intermediates, using cryogenic ion chemistry in conjunction with multiple resonance laser spectroscopy. Johnson was born and in Oakland, California in 1954 and raised in the San Francisco Bay Area. He graduated from the University of California at Berkeley with a degree in chemistry and from Stanford University in 1983 with a Ph.D. chemistry with Dick Zare. He was a postdoctoral fellow with Carl Lineberger at JILA/University of Colorado, Boulder, from 1983-1985 and joined the Yale faculty in 1985. He has served as Chair of APS Division of Laser Science and the ACS Division of Physical Chemistry, was co-editor of Ann. Rev. Phys. Chem. from 2012 to 2022, and is presently co-editor of the Annual Review of Physical Chemistry.

The 2024 SWRM PLENARY LECTURES

GOOCH-STEPHENS HONOREE - TUESDAY

Professor Andrew Ellington
Nancy Lee and Perry R. Bass Regents Chair in Molecular Biology
Wilson M. and Kathryn Fraser Research Professorship in Biochemistry

Department of Molecular Biosciences
The University of Texas at Austin

"Is a Blind Watchmaker the Same as a Blind Neural Net?"

5:45 pm Tuesday October 22
McLennan Hall, Waco Convention Center

Reception 5pm MONDAY
Hilton 3-Rivers Ballroom

Award Lecture

IS A BLIND WATCHMAKER THE SAME AS A BLIND NEURAL NET?

5:45-7 pm Tuesday October 22, 2024

McLennan Hall, Waco Convention Center

The Gooch-Stephens Lectures are an annual event of the Department of Chemistry & Biochemistry at Baylor University, and honor two former Chairs of the Department – Dr. W.T. Gooch and Dr. W.R. Stephens. The Department is pleased to announce that Dr. Andrew Ellington is one of two 2024 Gooch-Stephens Lecturers.

Dr. Andrew Ellington received his B.S. in Biochemistry from Michigan State University in 1981, and his Ph.D. in Biochemistry and Molecular Biology from Harvard in 1988. His post-doctoral work was with Dr. Jack Szostak at Massachusetts General Hospital, where he developed methods for the in vitro selection of functional nucleic acids and coined the term 'aptamer.' He originally received the Office of Naval Research Young Investigator, Cottrell, and Pew Scholar awards, and later was a Vannevar Bush Faculty Fellow of the DoD and a Howard Hughes Professor. Dr. Ellington's lab works centers on the development of nucleic acid circuitry for point-of-care diagnostics, on accelerating the evolution of proteins and cells through the introduction of novel chemistries, and on machine learning methods for engineering proteins and understanding evolutionary landscapes.

About the Gooch-Stephens Lecture Series

The Gooch-Stephens Lectures were established as a permanent annual event in recognition of the outstanding contributions of two longtime, highly respected chemistry professors and former department chairmen. Dr. W.T. Gooch became an instructor at Baylor University in 1908 after receiving two degrees from Baylor. His mentor was E.E. Reid, who later became an internationally known chemist at Johns Hopkins University. Dr. Gooch received his doctor of philosophy degree from the University of Chicago, where he studied with such eminent chemists of that day as Nef and Stieglitz. Dr. Gooch was especially known for his organic chemistry courses, which were taken by all chemistry majors and premedical students. From 1909 to 1949, Dr. Gooch served as chairman of the chemistry department at Baylor University. He died April 21, 1973, at the age of 87. Dr. W.R Stephens, who joined the Baylor faculty in 1922, came to Baylor from Meridian College where he had been dean. Dr. Stephens received his bachelor's and master's degrees from Auburn University and completed his Ph.D. at the University of Iowa, where he was associated with some of the best known chemists of that period. Dr. Stephens succeeded Dr. Gooch as chairman of the department in 1949. As chairman, Dr. Stephens enlarged the staff of the chemistry department and, in 1952, initiated and developed the doctor of philosophy program in chemistry. While chairman, Dr. Stephens devoted much of his energy and talents to the details of construction during the building of our former facilities in the Marrs McLean Science Building. He died Jan. 10, 1988, at the age of 95.

Previous Gooch-Stephens Awardees

1970 Professor Irving M. Klotz
1971 Dr. Byron Riegel
1972 Professor Harry B. Gray
1974 Professor Melvin Calvin
1975 Professor Herbert C. Brown
1976 Professor Willard E. Libby
1977 Professor Glenn T. Seaborg
1978 Professor E. J. Corey
1980 Professor Wm. N. Lipscomb, Jr.
1980 Professor Henry Taube
1982 Dr. Rosalyn Yalow
1983 Professor llya Prigogine
1983 Professor Roald Hoffmann
1985 Professor Neil Bartlett
1986 Professor F. A. Cotton
1986 Professor Bruce Merrifield
1987 Professor Derek Harold Barton
1988 Professor Paul C.W. Chu
1989 Professor Johann Deisenhofer
1991 Professor Allen J. Bard
1991 Professor Yuan T. Lee
1992 Professor M. Frederick Hawthorne
1993 Professor Per–Olov Löwdin
1994 Professor Kyriacos C. Nicolaou
1995 Professor Tobin J. Marks
1996 Professor Richard N. Zare
1997 Professor R.E. Smalley
1998 Professor Robert G. Bergman
1999 Professor F. Sherwood Rowland
2000 Dr. Ahmed H. Zewail
2001 Dr. K. Barry Sharpless
2002 Dr. Robert H. Grubbs
2003 Prof. Alan MacDiarmid
2004 Dr. Charles P. Casey
2005 Dr. Barry M. Trost
2006 Dr. Stephen J. Lippard
2007 Sir Harold W. Kroto
2008 Sir J. Fraser Stoddart
2009 Professor Omar M. Yaghi
2010 Professor Nathan S. Lewis
2013 Professor Donald R. Blake
2015 Professor Kendall N. Houk
2016 Professor Jon Clardy
2017 Professor Steven G. Boxer
2019 Professor Geraldine Richmond
2020 Professor Scott McLuckey

DETAILED TECHNICAL PROGRAM

SUNDAY MORNING

Computational and Theoretical Chemistry

K. L. Shuford, *Organizer, Presiding*

Texas 116

7:50 Introductory Remarks.

8:00 1. Probing the effects of size and charge on the hydration motifs of polyatomic anions. **G.S. Tschumper**

8:30 2. Getting (electronically) excited about computing vibrational spectra. **R.C. Fortenberry**

9:00 3. Tensor factorization methods in quantum chemistry. T. ZHAO, M. Simons, **D. Matthews**

9:30 4. Modeling strongly correlated electrons with stochastic and active-space-free approaches. **J. Shee**, D. Danilov, B. Ganoe

10:00 Coffee Break.

10:30 5. Uranium compounds: Seen through the eyes of quantum chemistry. **E. Kraka**

11:00 6. Adventures in computational chemistry: From rare-earth to transition-metal bonds, through noncovalent control of transition metal methylidene coupling, to magnetic interactions in a four-spin transition-metal tetramer. **M.B. Hall**

11:30 7. Creation of charge transfer states for photocatalytic water splitting in doped graphitic carbon nitride. **H. Lischka**, L. Ueno, L. Ferrao, F. Machado, L. Silva, L. Fonseca, A. Aquin

Advances in Organic Synthesis and Catalysis

L. Romero, J. L. Wood, *Organizers, Presiding*

Texas 115

8:00 8. Reprogramming organolithiums to access remote synthetic landscapes. **A.A. Thomas**

8:30 9. Strategies and Mechanistic Tools for Light-Mediated Organic Synthesis. **S. Pitre**

9:00 10. Hybrid Pd-radical chemistry: new mechanism, new possibilities. **V. Gevorgyan**

9:30 11. Synthesis and applications of fluorescent polymers in real-time by fluorogenic radical polymerization. **C.B. Cooley**

10:00 Coffee Break.

10:30 12. Target identification, molecular pharmacology, and medicinal chemistry of orphan cytotoxins. **J.K. De Brabander**

11:00 13. Overview of agricultural R&D at FMC. **T. McMahon**

Electron, Optical, Scanning, and X-ray probes for Materials Characterization and Science

J. Larson, *Organizer, Presiding*

Texas 118

8:30 14. X-ray Vision for A Macro-to-Nano Zoom through the Hierarchy of a Lithium-ion Battery. **Y. Liu**

9:15 15. Optothermal manipulation for materials characterization. **Y. Zheng**

10:00 Coffee Break.

10:30 16. Scanning Probe Microscopy: Designing interfacial surface chemistry to enable spatially selective patterning of proteins and DNA at the nanoscale. **J.C. Garno**, A.R. Walker, Q. Do

11:00 17. Generation of energetic hot electrons and superradiance from strongly quantum-confined perovskite quantum dots and their superlattices. **D. Son**

11:30 18. Initial carbonation of Ni(111) surfaces from carbon monoxide. **F. Xu**, J. Sanchez, B. Lamichhane, S. Kattel

Stone Symposium: Unusual Structure, Reactivity, and Properties of Inorganic Species

C. Martin, S. Yruegas, *Organizers, Presiding*

Texas 113

8:45 Opening Remarks.

9:00 19. On the interaction of carbenium ions with group 15 and 16 main group moieties. **F.P. Gabbai**

9:25 20. Perturbing electron density within Al-H-Ni subunits in heterometallic nickel-aluminum hydride complexes. **M. Shoshani**

9:50 21. Oil & water: Mixing heavy 5p/6p donor sets with late 3D metals for enhanced easy axis anisotropy. **M.J. Rose**

10:15 Coffee Break.

10:35 22. Main group atoms in coordination chemistry. **T. Tilley**

11:15 23. Heteroleptic Copper(I) charge-transfer photosensitizers supported by β-Diketiminates. D. Kim, **T.S. Teets**

11:40 24. A one-pot synthesis of Mo^0 and W^0 complexes as Olefin Metathesis catalyst precursors. **Y. Ning**

Bioinorganic Chemistry

P. J. Farmer, *Organizer, Presiding*

Texas 114

10:30 25. Cuprotosis and the DSF/Cu reaction. **P.J. Farmer**, J. Lyons

11:00 26. Mechanistic insights into non-heme iron thiol dioxygenase activity. **J. Li**, R. Duan, Y. Wang, I. Davis, A. Liu

11:30 27. Glycerol-dependent conformational activation of cysteamine dioxygenase (ADO) revealed by EPR spectroscopy. J. Helms, M. Probst, J. Paris, M.P. Hendrich, **B.S. Pierce**

SUNDAY AFTERNOON

Advances in Organic Synthesis and Catalysis

L. Romero, J. L. Wood, *Organizers, Presiding*

Texas 115

1:00 28. Palladium-catalyzed aminoboration of alkenes. **K. Hull**

1:30 29. Natural products in the atmosphere. **R.J. Thomson**

2:00 30. Total synthesis of complex, bioactive natural products. **C.D. Vanderwal**

2:30 31. Strained Intermediates and Chemical Education as Vehicles for Innovation.. **N.K. Garg**

3:00 Coffee Break.

3:30 32. Complex natural products as a driving force for discovery in organic chemistry. **B.M. Stoltz**

4:00 33. Stereoselective reactions with feedstock chemicals. **U.K. Tambar**

Biochemistry (General)

L. R. Marshall, *Organizer, Presiding*

Texas 117

1:00 Introductory Remarks.

1:00 34. Exploring CRISPR-Cas9 HNH-domain catalyzed DNA cleavage using accelerated quantum mechanical molecular mechanical free energy simulations. **R. Van**, X. Pan, J. Liu, P.K. Agarwal, B. Brooks, R. Rajan, Y. Shao

1:20 35. Synthesis and evaluation of carbamate bioconjugates for hepatocyte modification. **J. Karunananthan**, E. McGown, R.R. Kane

1:40 36. NitrOFF: A fluorescent biosensor to visualize nitrate transport in living cells. **M. Cook**, K. Ji, S. Phelps, J. Tutol, S. Dodani

2:00 37. Surfactant assisted protein encapsulation in ZIF-8 MOF. **R.N. Hudson**, R. Ravanfar

2:20 38. Applying universal design to make chemistry more accessible to those with visual impairment. **L. Garza**, B.F. Shaw

2:40 39. Unlocking pHLIP's dynamic transformations using 2D IR spectroscopy. **R. Antonelli Maia**, C. Baiz

3:00 Break.

3:25 40. Targeting phosphatidylserine in the tumor microenvironment with cathepsin B and L cleavable antibody/betabody drug conjugates (ADCs)/(BDCs). **Y. Deng**, J. Ford, J. VanNatta, C.J. Maguire, D. Mondal, N. Phinney, R.A. Brekken, K.G. Pinney, M.L. Trawick

3:45 41. Development of Macrocyclic Organo-Peptide Hybrids for targeting HIV-1 Nef protein function. **P. Agredo Sanin**, K. Wang, A. Saseendran, X. Jia, R. Fasan

4:05 42. Developing an anti-superoxide dismutase 1 (SOD1) aptamer for tracking SOD1 migration and aggregation in neurodegenerative diseases. **A. Pham**, G. Stovall

4:25 43. Selective capture, isolation, and characterization of mucin foraging neuraminidase-active bacteria from microbiomes using a non-inhibitory activity-based probe. **K. Shipman**, A. Steiger, E. Ugwuoji, L. Webber, A. Anand, A.T. Wright

4:45 Closing Remarks.

Bioinorganic Chemistry

P. J. Farmer, *Organizer, Presiding*

Texas 114

1:00 44. NO hidden electrons: Bioinspired redox- and spin-active transition metal coordination complexes based on Nitrosylated-Fe-N2S2 metalloligands. **M.Y. Darensbourg**

1:30 45. Kinetics-based luminescence methods for monitoring and quantifying peroxynitrite and HNO. **A.R. Lippert**

2:00 46. Electron transfer sequence in NO reduction: HNO and N_2O as signaling outputs. **P. Ghosh**, T.H. Warren

2:30 47. Recent Progress in Biosynthetic Modeling of Metalloenzymes. **Y. Lu**

3:00 Coffee Break.

3:30 48. Improving the drug-like properties of a potent antioxidant scaffold for treatment of Alzheimer's and other neurodegenerative diseases. **K.N. Green**

4:00 49. Light triggered metallodrugs for Cancer therapy. **S.A. McFarland**

4:30 50. Fluorescent sensors for metalloenzyme active sites: applications in antibiotic resistance and beyond. **E.L. Que**, S. Price, D. Hudson, A. Malto

Computational and Theoretical Chemistry

K. L. Shuford, *Organizer, Presiding*

Texas 116

1:00 51. Can noise enhance quantum coherence?. **E.R. Bittner**

1:30 52. Plumbing potentials for molecules with up to tens of atoms: How to find saddle points, fix leaky holes, build hole-free PESs, and find CI seam minima. **B. Poirier**, R. Liang, M. Aarabi, A. Pandey

2:00 53. Mesoscale quantum dynamics in molecular materials. **D. Raccah**

2:30 54. Cavity modified exciton transport. **A. Mandal**

3:00 Coffee Break.

3:30 55. Dispersion, from a major to a minor component in intermolecular forces, plays a critical role in material properties. **F. Wang**

4:00 56. Incorporating nuclear quantum effects into non-adiabatic molecular dynamics. **F.A. Shakib**

4:20 57. Atomistic quantum dynamics simulations for vibrational spectroscopy. **M. Momenitaheri**

Materials for Energy and Environment

Cosponsored by ENFL

J. Larson, *Organizer, Presiding*

Texas 118

1:00 58. Plasmonic photocatalysis with antenna-reactor nanoparticle complexes. **N.J. Halas**

1:30 59. Ternary Oxide Semiconductors and Alloys. **R. Krishnan**

2:00 60. Understanding the Interplay of Singlet Fission and Exciton Transport in Organic Crystals. **S.T. Roberts**

2:30 Coffee Break.

3:00 61. Varied polyanionic dimensionality, complex structures, and thermoelectric properties in the Eu-Zn-As ternary system. **S. Baranets**

3:30 62. Lone but not alone: Modulating the energy positioning of lone-pair-derived states for the design of photocatalytic architectures. **S. Banerjee**

4:00 63. Tailoring Spin Configurations and Mass Transfer in Molecular and Framework Catalysts for Superior Oxygen Electrocatalysis. **S. Sreenivasan**

4:30 64. Hydrogen evolution and oxygen reduction on varied OH/F-terminations of $Ti_4N_3T_x$ Nitride MXene. **A. Djire**

Undergraduate Symposium

J. R. Ingle, *Organizer, Presiding*

Ranger 106/107

1:00 Introductory Remarks.

1:05 65. Templated synthesis of strained OBO-doped aromatic macrocycle. **M. Bilal**, V. Espinoza Castro, A. Slobin, A. Valles, R. Hernandez Sanchez

1:20 66. Reactions of dodecacarbonyltriosmium with substituted pyrazoles. **J. Polk**, N. McKinney, N. Palomino, C.B. Powell, G.L. Powell

1:35 67. Highly emissive zero-dimensional hybrid antimony chlorides A_2SbCl_5 featuring long-chain cations. H. Majumder, **A.A. Miranda**, K. Thanabalasingam, K. McCall

1:50 68. *En route* to a molecular polygon with square geometry containing four platinum vertices and four (C≡C) edges. **T.M. Jackson**, A.J. Perez, J.A. Gladysz

2:05 Intermission.

2:10 69. *Withdrawn*

2:25 70. *Withdrawn*

2:40 71. Triple-barrel capillary interfacial microreactor for reaction acceleration. **J. Kim**, M.E. Edwards, D.P. Freitas, W.J. Oluwasegun, L.A. Baker, X. Yan

2:55 Coffee Break.

3:20 Introductory Remarks.

3:25 72. Investigation of photophysical and hydrodynamic properties of fluorescent probe molecules in aqueous and reverse micelle environment. **D. Kim**, M. Opolz, R.K. Nayak

3:40 73. Unlocking nature's secrets: Method development and LC-MS troubleshooting for discovering bioactive compounds in herbal plants. **J. Thorne**, L. Hunter, K. Priyasantha

3:55 74. Unveiling bioactive phenolics: Identifying key compounds in herbal tea samples. **L. Hunter**, J. Thorne, K. Priyasantha

4:10 Intermission.

4:15 75. Determination of caffeine and ascorbic acid content in kombucha using UV-visible spectrometry and multivariate regression modeling. **A. Gaudard Correa Rangel**, J.R. Ingle

4:30 76. Detection of BPA in clothing using flourescence spectrophotometry. **B. Steinfeldt**, S.E. Hubbard

4:45 77. Preparation of antibiotic-chitosan conjugate hydrogels for wound care applications.. **A. Browning**, S.K. Hamilton

Mass Spectrometry for Biomolecules

E. S. Gallagher, *Organizer, Presiding*

Lone Star 104

1:30 78. The disordered acidic domain of Asf1 regulates Rtt109 acetylation of H3-H4. **S. D'Arcy**

2:00 79. Top down proteomics reveals a proteoform-truncation mechanism that supersedes the DNA damage and apoptotic response.. F.M. Joseph, **N.L. Young**

2:30 80. Neuropeptide analysis to explore potential mechanisms of alcohol addiction in rats. **M. Asokan**

3:00 Coffee Break.

3:30 81. Water plays key roles in the stabilities and compositional entropy of mutant transthyretin tetramers. **C. Lantz**, R. Rider, S. Yun, A. Laganowsky, D.H. Russell

4:00 82. Capturing RAS oligomerization on a membrane. S. Yun, **E. Scott**, J. Chang, H. Bahramimoghaddam, M. Lynn, C. Lantz, D.H. Russell, A. Laganowsky

4:30 83. Interfacial electromigration for analysis of small volume biofluid. **M.E. Edwards**, D.P. Freitas, E.A. Hirtzel, N. White, H. Wang, L. Davidson, R.S. Chapkin, Y. Sun, X. Yan

Stone Symposium: Unusual Structure, Reactivity, and Properties of Inorganic Species

C. Martin, S. Yruegas, *Organizers, Presiding*

Texas 113

1:45 84. *In crystallo* synthetic chemistry. **D. Powers**

2:10 85. Facile access to organostibines via selective organic superbase catalyzed antimony-carbon protonolysis. **C. Krempner**

2:35 86. Synthesis and oligomerization reactivity of tetrylaminoboranes. **C. Wagner**

3:00 Coffee Break.

3:20 87. Bis(carbene) scaffolds for the encapsulation of multimetallic complexes. **S. Yruegas**, M. Bhandari

3:45 88. Reactivity of Lewis Superacidic (*ortho*-Carboranyl)boranes. **M. AKRAM**, J.R. Tidwell, J.L. Dutton, C. Martin

4:10 89. Reactivity of the dimesityl-1,8-naphthalenediylborate anion with dipolarophiles. **T. Hudnall**, J. Wang

4:35 90. Acyclic diaminocarbenes: Organometallic adventures with an unusual ligand class. **L.M. Slaughter**, M. Ellison, J. Nguyen, D. Vargas Trujillo

SUNDAY EVENING

Dial-Black Award Lecture

L. Romero, *Organizer, Presiding*

McLennan Hall

5:45 Introductory Comments.

6:00 91. Translational science: The chemistry-biology-medicine continuum. **P.A. Wender**

6:55 Dial-Black Award.

POSTER SESSIONS and EXPO and GRADUATE FAIR and RECEPTION

Brazos Ballroom

7:00 - 9:00 pm

Biochemistry Poster Session

L. R. Marshall, *Organizer*

92. Development of a rapid lateral flow assay targeting RC0497 for timely diagnosis of severe tick-borne spotted fever rickettsioses. **Y. pal**, R.C. Willson, D. Walker, K. Kourentzi, R. Fang, K. Brosamer

93. Effect of thyroxine on transthyretin mutant structure & dynamics monitored by native ion mobility mass spectrometry. **R.L. Rider**, C. Lantz, S. Yun, A. Laganowsky, D.H. Russell

94. Study of combretastatin A-4 release from the beta-galactosidase activated prodrug combretastatin A-4-beta-D-galactopyranoside. **A.M. Atoki**, C. Pavlich, Q. Scott, S. Anliker, M. Krayevsky, K.G. Pinney, M.L. Trawick

95. Mechanism of action of a series of OXi8006 analogues in MDA-MB-231 cells. **W.K. Rathnayake**, Y. Deng, C. Tamminga, Y. Wong, K.G. Pinney, M.L. Trawick

96. Advanced forensic chemistry: Assessing the susceptibility of imported and domestic rice varieties to bio-agent threats using escherichia coli models. **V. Gonzalez**, D. Wilson, H. Sharifan

97. Identification of cadmium as a structural and functional modulator of PSD-95 regulating NMDARs at postsynaptic membranes. **C. Garza**, Y. Zhang

98. *In vitro* Investigation of Dimethyl Disulfide, a metabolite of the cyanide antidote candidate Dimethyl Trisulfide. **A. Khurana**, **K. Gonzalez**, I. Petrikovics, D.E. Thompson

99. N-acyl taurines, related sulfonates, and acyl amino acid substrates of P450 Cytochromes. **A. Alencar**, **D. Gilils**, Y. Figueroa Flores, D.C. Haines

100. Exploring the antioxidant properties of watercress and mint extracts in serum albumin protein under oxidative stress. **N. . Aziekwu**, P. Tovar, T.T. Dao, B. Sengupta

101. Naloxone derivatives to improve the opioid crisis. **M. Garcia**

102. Effects of exogenous hormone replacement therapy and in a hypothyroid, post-menopausal rat heart failure model. **E. Eversole**, M.M. Bowden, B. Fallon, F. Naegele, A. Martino, A. Lu, S. Schmidt, R.C. Willson, A. Bhimaraj, K. Youker, C.S. Filgueira

103. Utilizing unsaturated fatty acids as bacterial inhibitors to act as a natural preservative in eye drops. **V. Ramos**, B. Blair

104. *Withdrawn*

105. Engineering *Escherichia coli* for *Enterococci faecalis* penicillin binding protein 4/5 expression and the creation of nanodiscs. **M.M. Bowden**, K.M. Hood, A.P. Streling, W.R. Miller, C.A. Arias, C.S. Filgueira

106. Role of Fe-Doping of ZnO on Antibacterial Action. **J. Brannon**, D. Johnson, R. Cuth, Y. Strzhemechny

107. Calcium-dependent chemiluminescence catalyzed by a truncated c-MYC promoter G-Triplex DNA. **M.W. Myhre**, **M.K. Das**, E.P. Williams, W.M. David, S.M. Kerwin

108. Transcriptomic signature in the immune response to respiratory sensitizers using an alveolar model and database analysis. **T. Jefferis**, K.L. Griffin, J. Liu, M. Gibb, C.M. Sayes

109. Replisome decoupling between Alpha and Tau subunits in the Pol III holoenzyme cause reduced cellular fitness and genomic instabilities in *E. coli*. **M. Welikala**, **L.J. Butterworth**, M.S. Behrmann, M.A. Trakselis

110. Oxidative stress modulates mitochondrial transcription factor A (TFAM) binding to DNA. **R. Sharkey**, Y. Gao

111. Cadmium binding with the N-terminus of synapse associated protein 102 and implications for its postsynaptic functions. **C.H. Morales Alba**, Y. Zhang

112. Predicting chemical respiratory sensitizers with machine learning QSAR models. **K.L. Griffin**, J. Liu, T. Jefferis, J. Peeples, C.M. Sayes

113. Function-oriented profiling of mucin degradation in the gut microbiome. **S.J. Joseph**, A.T. Wright

114. Regulation of the pyrimidine ribonucleoside pathway in *Pseudomonas putida*. S. Fatima, K.B. Young, **T.P. West**

115. Xylitol synthesis by *Candida guilliermondii* on a plant biomass hydrolysate. **E.O. Brefo**, T.P. West

P003. Elucidating extracellular electron transfer in *Lactiplantibacillus plantarum* for bioelectronics. **R. Alba**, B. Blackburn, V.O. Porokhin, A. Hatch, S. Hassoun, C. Ajo-Franklin, E. Mevers

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Undergraduate Symposium Poster Session

J. R. Ingle, *Organizer*

116. DFT mechanistic investigation of aryne insertion into boron compounds. **M. Mora**, J.E. Dannatt, P. Patel

117. Small Molecule Proprotein Convertase Subtilisin/Kexin Type 9 (PCSK9) inhibitor for anti-platelet activity for the treatment of stroke. **S. Palakurthi**, M. Thalla

118. RNA-Based Aptamers for the Detection of B Cells as Biomarkers in Diabetes. **I. Batta**, G. Sharma

119. *In silico* analysis of RNA-based aptamers for interaction with CD19 receptor in CAR-positive T-Cell enrichment and monitoring. **F. Pachloo**, G. Sharma

120. *In silico* analysis to predict inhibitors against integrin receptor. **V. Sharma**, G. Sharma

121. **MOVED to P002 (Tuesday Poster Session)** Targeted Inhibition of SARS-CoV-2 Main Protease (Mpro) Using Proteolysis Targeting Chimeras (PROTACs). **K. Chidambaranathan**, G. Sharma

122. Computational analysis for identifying effective therapeutics for malignant melanoma. **M. Krishna**, G. Sharma

123. Computational analysis of cardiac disease protein biomarkers using aptamers. **T.S. Vinapamula**, G. Sharma

124. *In silico* analysis of γδ TCR-enhanced CAR T-Cell therapy for Metastatic Prostate Cancer. S. Adapa, **G. Sharma**

125. *In silico* analysis RNA-based aptamers in neuroblastoma diagnosis and targeted therapy. **K. Patel**, G. Sharma

126. Preparation of highly purified osajin and testing in pancreatic tumor cell proliferation assays. L. Reynolds, A. Wood, E. Soward, R. Srinivasan, **W.L. Whaley**

127. Osajin is preferentially extracted from Osage orange fruit tissue in a hexane fraction that contains very little pomiferin. J.B. Dulaney, E. Erdmann, A. Trammell-Coburn, **W.L. Whaley**

128. Study of properties and reactivity of curcumin. **E.E. Frazier**, G.S. Garusinghe

129. Interactions of curcumin with metal (Pt, Au) complexes. **E.E. Frazier**, G.S. Garusinghe

130. High throughput virtual screening for transition state inhibitors of ATP-Citrate Lyase. K. Hensley, **E.R. Hensley**

131. Zero extraction force dies for gummy metals or brittle ceramic pellets. **A. Kojima**, C. Jenny, M. Gott, M. Zach

132. Exploring surface-mediated formation of hydrogen peroxide in levitated microdroplets. **E.R. Hamilton**

133. FTIR analysis of microplastics in fingerprints. **O. Barclay**, **J.D. Beatty**

134. Computational investigation of the effects of post translational modifications and cancer mutation on PARP-2. **B. Hughes**, G.A. Cisneros

135. Synthesis of iodonium salts and investigation of aryne reactivity with boron-oxygen functionalities. **J.B. Nelson**, J.E. Dannatt

136. Investigation of electronic and hydrodynamic properties of fluorescent Texas red dyes in reverse micelle environment. **D. Kim**, N. Moro, R.K. Nayak

137. Fluorescence quenching and photophysics of Alexa Fluoro (AF) 647 dye by graphene oxide nanoparticle in aqueous and confined reverse micelle environment. **W. Johnson**, N. Moro, D. Kim, R.K. Nayak

138. Analysis of aqueous phosphate solutions by conductometric titration in the presence of sulfate. **L. Jackson**, L.D. Schultz

139. Extraction, isolation, and characterization of gaillardin and its effectiveness as a histone deacetylase inhibitor. **N. Pyenta**, P. Pyenta, H. Shin

140. Removal of pharmaceuticals from water using plant-based polymers. **M. Fowler**, R. Srinivasan

141. *Withdrawn*

142. Covalent modification of vascularized tissue. **S. Thatcher**, J. Karunananthan, R.R. Kane

143. Synthesis and Characterization of Light-Absorbing (3,5-difluoro-2-(pyridin-2-yl)phenyl)platinum(II) Complexes with Xanthate Ligands. **M. Mason**, B.W. Smucker

144. Synthesis of Kobayashi precursors and exploration of aryne insertions into trimethyl borate. **M. Zeaa**, J.E. Dannatt

145. The aryne insertion into the boron-chlorine bond and effect of common extraction solvents on reaction crudes. **A. Sharma**, S. Berzhanskaya, J.E. Dannatt

146. Determination of Hammett sigma values for 3-carboxyphenyl boronic acid and 4-carboxyphenyl boronic acid. **K.E. George**, M. Bielinski, J.E. Dannatt

147. Prodrugs of vascular disrupting agents activated by β-galactosidase to target the tumor microenvironment. **Q. Scott**, C. Pavlich, S. Anliker, M. Krayevsky, A.M. Atoki, B. Afzal, L. LIU, R.P. Mason, M.L. Trawick, K.G. Pinney

148. PFOA degradation by molecularly inspired porphyrin-based heterogenous electrocatalyst. **B.A. Dorsey**, N. Ocuane, J. Calvillo, D. Villagran

149. Microbial metal miners: nicotianamine synthase in *Fusobacterium varium* metallophore biosynthesis. **O.E. Hernandez Reyes**, K. Meneely, A. Lamb

150. Complexation of Uranyl (VI) onto monohalogenated Schiff-base salophen Ligandsl. **L. Ozer**, J. Ducilon, D.M. Eralie, A.E. Gorden, J. Gorden

151. Pharmacophore-directed retrosynthesis applied to talaromynoid H: A model study of the late stage installation of the allylic epoxide bearing tricyclic core. **P. Junghans**, A. Youman, D. Romo

152. Enhancing stability of L-ascorbic acid in cosmetic formulations: The synergistic role of ferulic acid analyzed via HPLC and iodine oxidation. **J.A. Klein**, C. Burnett

153. Analyzing the degradation rates of natural polymer-based novel materials for use in biomedical applications. **T. Smith**, S.K. Hamilton

154. Syntheses and characterization of platinum(II) complexes with 3-phenylisoquinoline and xanthate or dithiolene ligands. **C. Samonte**, B.W. Smucker

155. Oxidation of antimony halide with ortho-quinones. **A.C. Mehnert**, F.P. Gabbai

156. Region specific protein profiling of heart tissue using bottom-up proteomics. **S.C. Beno**, **G.Z. Atanasova**, K. Wilhelm, R.A. Villacob, T. Solouki

157. Photochemical oxidation of nitroaromatic heterocycles in the environment. **N. Kondapalli**, A.W. Harrison

158. Atmospheric photochemistry of brown carbon from wheatgrass wildfire. **O.A. Cernero**, A.W. Harrison

159. Making a phase diagram: Differential scanning calorimetry in an inert environment. **S. Smith**, M. Plata, J. Chan

160. Improved synthesis of C_2 spaced organogelators. **A. Toombs**, A.J. Carr

161. Expression and reactivity of phenylacetone monooxygenase (TfPAMO) from *Thermobifida fusca*. **S.M. Reyes**, M.E. Hinze, C.T. Ammermann

162. Slow but steady RuBisCO: Utilizing a recombinant RuBisCO to inform optimization. **A. Paul**, Z. Hoffpauir, K. Meneely, A. Lamb

163. Optimizing and tailoring machine learning models to predict pK_a. **M. Meduna**, P. Patel

164. Synthesis and electrochemistry results of Diethyl-2-[3-nitrophenylmethylene]malonate and Diethyl-2-[4-nitrophenylmethylene]malonate. **G. Linthicum**, I. Hotsuliak, C.A. Hansen, J. Shao

165. Exploring new structural features in organogelation. **L. Butler**

166. Characterizing alkoxy-substituted quadrupolar fluorescent dyes. **S. Mason**, J. Lancaster, A. Lim

167. Enantioselective *syn*-aldol reactions of *N*, *N*-dimethylphenylacetamides. **A. Square**, **P.B. Chanda**

168. Study of iodine distribution and concentrations in western Oklahoma brine waters and recycling of used chloroform. **J.R. Wickham**, D. Edlin

169. Recyclable and water-soluble Cu(II)-Schiff base complex: green catalyst for C-H activation reactions. M. Guagliardo, **X.D. Duke**, A.E. Gorden

170. Boron-mediated diastereo- and enantioselective aldol reactions of arylacetates. **P. Le Riche**, **P.B. Chanda**

171. An efficient diastereoselective synthesis of *syn*-*β*-hydroxy-*α*, *β*-diaryl carboxylic acid esters. **S. Lee**, **P.B. Chanda**

172. Synthesis of prochiral substrates for the selective access of α-acyloxy ketone scaffolds. **R. Carter**, M.E. Hinze

173. Photooxidation prevents aggregation of amyloid-β peptides. **C. Rider**, U. Umezaki, A. Martí

174. Chemical desymmetrization of trehalose with high efficiency. **A. Drake**, D. Czapski, M. Mulkey, J.A. Buonomo

175. Elucidating the catalytic properties of molecular transition metal dichalcogenides for O_2 activation and subsequent conversion of methane to methanol. **T. Jaber**, K.A. French, K.L. Shuford

176. Utilization of retro-cope elimination reaction as a rapid bioorthogonal reaction and application in the metabolic engineering of trehalose glycolipids in *Mycobacteria*. **M. Mulkey**, D. Czapski, A. Drake, J.A. Buonomo

177. Expressing protein in beta-2-microglobulin. **D. Carrillo**, J. Richardson

178. Investigating amyloid fibril cross-b sheet intermolecular interactions through b2m aggregation kinetics *in vitro*. **A.E. Nelson**, D. Carrillo, J. Richardson

179. Crosslinking transmembrane helices in subunit *a* and molecular docking of F1F0 ATP synthase. **B. Karnes**, E.A. Nalley, K.J. Moore

180. Protein purification of Beta-2-Microglobulin mutants. **L. Balderas**

181. Exploring dynamics of proteins in levitated microdroplets. **E. Aleman**

182. Investigating the antimicrobial properties of *Trichoderma viride* volatile organic compounds. **M. Bierschenk**, M. Kopecki-Fjetland

183. Synthesis of SAM towards engineering SAM synthases & methyltransferases for universal alkyl donation. **R. Srivastava**, J. Clinger

184. Synthesis and analysis of glucose-based tetrazole probe for profiling glucosidases in gut microbiota. **A. Pitts**, J. Russo, A.T. Wright

185. Effects of lichen and moss volatile organic compounds on the growth of *Neolentinus lepideus*. **A. Wheatley**, M. Kopecki-Fjetland

186. Synthesis of a photochromic bicyclic aziridine. **F. Tung**, C. Cu Castillo, P.D. Arche, M. . Stefan, M.C. Biewer

187. Towards the structural characterization of the FIrB PAS domain. **M.A. Rios**, K. Meneely, A. Lamb

188. Comparison of the alkene products formed from dehydrations of 1-benzylcycloalkanols. **S. Magallan**, B. Hathaway

189. Synthesis of remotely borylated aza-heterocycles. S. Bhatt, A.M. Nicely, C.U. Powell, **M. Huff**, S.B. Thibodeaux, Y. Wang, S. Vasylevskyi, K.L. Hull

190. Can hydrogen-bonded metal-organic frameworks (HBMOFs) mimic clay functionality?. **C. Gross**, G.A. Hogan

191. Comparison of different digestion protocols for studying the effects of chronic alcohol exposure in rat brain tissue. **V. Ng**, M. Asokan, L. Natividad

192. Developing sustainable polymer chemistry experiments using hydrogels. **M. Shareghi Borojeni**, E. Trufan, E. Bouhoutsos-Brown

193. Inclusion of pyridine molecules within a Cu-based hydrogen-bonded metal-organic frameworks (HBMOFs). **J. Bruyns**, G.A. Hogan

194. Creating a green curriculum using piezoelectric materials. **N. Nabavi**, E. Trufan, E. Bouhoutsos-Brown

195. Refining activity-based protein profiling in complex biological systems. **M. Andrews**, C. Nwike, A.T. Wright

196. Catalysis kinetics: Computational investigation of silica-supported zirconium catalysts. **A. Caranti**, P. Patel

197. Analysis of BPA leaching from feminine hygiene products into simulated vaginal fluid using fluorescence spectrophotometry. **M. Rettig**, S.E. Hubbard

198. Reactions of paraxanthine and saccharin with osmium carbonyl. **G.S. Sullivan**, A. Schumacher, G.L. Powell, C.B. Powell

199. Sweet vs. science: Influence of nonnutritive coffee syrups on Escherichia coli. **D. Komlofske**, A.D. Millsap

200. Enhancing student learning outcomes: The role of edutainment tools in undergraduate education. S. Bashir, J.C. Lawrence, **J.L. Liu**

201. Synthesis, biological evaluation, and molecular modeling of imidazoles to investigate structural activity relationships. E.A. Nalley, **S. Meraz**, J. Duran-Chaves, C. McClenan

202. Synthesis of β-keto carbonyl scaffolds and standards to investigate oxidation outcomes. **E. Bloss**, M.E. Hinze

203. Computational study of pesticide capture by metal-organic frameworks. **L. Guzman**, H. Chen

204. Synthesis and characterization of biologically compatible tetra-aza macrocyclic molecules to function as therapeutic agents for Alzheimer's disease. **S. Anjum**, S. Nilewar, K.N. Green

205. Assessing novel vascular disrupting agents in renal cell carcinoma by bioluminescence imaging. **S. Sun**, T. Wang, R. Vairin, K.G. Pinney, R.P. Mason, **L. LIU**

206. Synthesis of *N*–alkylated 2-aminobenzothiazoles using pyridinium bromide perbromide.. **P. Varma**, C. Martinez, S. Morris

207. Improving the cytoplasmic delivery and specificity of Trimethoprim via conjugation to enterobactin. **D. Amaegbo**, G. Kamyabi, E.M. Nolan

208. Synthetic pathways of azobenzene thiol cross-linkers for polysaccharides. **W. Woulfe**, W.J. Brittain

209. Standardizing the characterization of conductive hydrogels. **H. Garza**, A. Perry, R. Posey, J. Tropp

210. Analysis of branched-chain amino acids in GU Energy Gels. **J. Vega**, C. Burnett

211. Analysis of alkaloid profiles of *Mitragyna speciosa*, a tree with novel and paradoxical medicinal properties. **I. Mounteer**, C. Burnett

P007. Synthesis of chloropyridinol derivatives as possible histone deacetylase inhibitors (HDACi). **D. Abbott**, H. Shin, P. Pyenta

P008. Sample Preparation Towards Dynamic Structural Biology of SAMDC. **J.R. Patel**, J. Clinger

P009. Ionic Liquids as Surfactants. **C. Plaisance**, I. Eamon, J. Mcguire, V. Thalangamaarachchige

P011. A focused approach of enhancing the antioxidant and antidiabetic activities of silver nanoparticles synthesized using *Mentha piperita* and *Thymus schimperi* leaf extracts. **L. Stovall**, A. Geremew, L. Carson

P012. Enhancement of plant growth and nutritional quality using zinc oxide nanomaterials. **D. Guthrie**, A. Geremew, L. Carson

P013. Green synthesis of novel silver nanoparticles using *Aframomum corrorima* seeds: a focus on antioxidant and antidiabetic activities. **J. Graham**, A. Geremew, L. Carson

MONDAY MORNING

Chemical Reaction Kinetics, Dynamics, and Mechanisms

D. J. Bellert, *Presiding*

Lone Star 103

8:00 212. Quantum tunneling in the C-H bond activation of Ni+ mediated CH_3COOH decomposition. **G. Pinto**

8:20 213. Hydrogen tunneling without the typical large KIE measured in the mediated decay of the $Co(CH_3COOH)^+$ complex. **S.U. Okafor**, G. Pinto, M. Brdecka, W. Smith, D.J. Bellert

8:40 214. Illuminating nanomaterials: A thermodynamic study of chloride ion release from photolysis. **X. Chen**, D. Conrad, E.V. Anslyn, C. Baiz

9:00 215. Product state distributions and dissociation dynamics from ozone photolysis in the Huggins band via $O(^3P_J)$ VMI. **N. Shuber**, M. Fast

9:20 216. Temperature dependent kinetics for the reactions of $Ta^+ + CH_4$ and the successive higher order reactions. **T. Lewis**

9:40 217. Photodissociation of ozone in the Huggins Band: Measurements of O_2 $(a^1\Delta_g)$ rotational distributions. **M. Fast**, S.W. North

10:00 Intermission.

10:20 218. Theoretical insight into the dynamics of Co^+ and Ni^+ mediated decomposition chemistry of acetic acid. **H. Barzinmehr**, G. Pinto, S.U. Okafor, D.J. Bellert

10:30 219. How the kinetic signature of two-state reactivity (TSR) was determined. **D.J. Bellert**

11:00 220. Direct imaging studies of atmospheric photochemistry: Energetics, roaming, and forbidden processes. **S.W. North**

11:30 221. Temperature- and size-dependent, water-cluster-mediated long range proton transfer in microhydrated 4-aminobenzoic acid. **M.A. Johnson**

Computational and Theoretical Chemistry

K. L. Shuford, *Organizer, Presiding*

Texas 116

8:00 222. Towards affordable free energy simulations of enzyme reactions. **Y. Shao**

8:30 223. Dimensionality reduction analysis for biomolecular simulations. **P. Tao**

9:00 224. Accelerating QM/MM simulations with multiple time step and machine-learning approaches. **K. Nam**, A. Arattu Thodika, X. Pan, Y. Shao

9:30 225. Development of multiscale simulation approaches for the characterization of photochemical reactivities in biomolecules. **R. Liang**

10:00 Coffee Break.

10:30 226. Simulating protein association and aggregation. M. Sheridan, A. Chesney, M. Punchi Hathanalage, **U. Hansmann**

11:00 227. Quantifying Allosteric Response using ShapeGMM. **M. McCullagh**

11:30 228. Unraveling protein-protein dissociation via atomistic simulations. **O. Valsson**

DNA Damage Detection, Tolerance, and Toxicity

Cosponsored by TOXI
M. A. Trakselis, *Organizer, Presiding*

Texas 117

8:00 229. DNA damage at sites of terminated transcripts. **S. Rosenberg**

8:30 230. ATPase activity is essential but insufficient for mitochondrial DNA replisome function. **Y. Whitney**

9:00 231. DNA polymerase kappa supports replication gap suppression in glioblastoma cells through a mechanism involving fork reversal factors. **R.L. Eoff**

9:30 232. Polyethylene terephthalate (PET) microplastics and nanoplastics induce cytotoxicity in MCF-7 cells. **Z. Kasuske**, P. Roy, K. Arole, J.E. Canas-Carrell, K. Singh

9:45 Break.

10:15 233. Novel mechanisms of genetic instability in Cancer. **K. Vasquez**

10:45 234. Tyrosine phosphorylation of RAD51 controls its structure and function at the break.. **E. Dray**

11:15 235. Mitotic activation of the Fanconi anemia pathway induces chromothripsis and ecDNA formation. J. Engel, **P. Ly**

Electrochemical Interfaces Relevant to Energy and Environment

Cosponsored by ENFL
J. Larson, *Organizer, Presiding*

Texas 118

8:00 236. Hydrogen-bond environments at an electrochemical interface: insights from IR spectroscopy and MD simulations.. **C. Baiz**

8:30 237. Standardizing the Characterization of Conductive Hydrogels. **J. Tropp**

9:00 238. Electrochemical synthesis of formamide from CO_2 using Titanium Nitride (Ti_2N) MXene. **A. Djire**

9:30 239. Electrodeposition of aluminum from phenoxide-based binary electrolyte solutions. D.J. Mosman, C. Silguero, A. Ambar, J. Antonetti, **M.L. Aubrey**

10:00 Coffee Break.

10:30 240. Electrocatalytic reduction of nitrate to ammonia at oxidized vanadium surfaces with V (3+) and V (4+) oxidation states. **Q. Adesope**, M. Altafi, S. Amagbor, V. Mesilov, K. Jeffry

11:00 241. Interface-modulated kinetic differentials as a key design principle for redox photocatalysis by Sb_2VO_5/QD heterostructures. **J. Ayala**, K. Garcia-Pedraza, A. Giem, U. Wijethunga, S. Hariyani, J.L. Carrillo, D. Watson, S. Banerjee

11:30 242. *Operando* Infrared Nanospectrosocpy of Electrochemical Interfaces. **J. Larson**, Y. Lu, A.I. Baskin, X. Zhao, P.D. Ashby, D. Prendergast, H. Bechtel, R. Kostecki, M. Salmeron

High School Educators Symposium

A. Chu, *Organizer*
M. C. De Mesa, K. Moos, *Presiding*

Ranger 110

8:00 Registration (on-site).

8:30 Symposium Introduction/Trivia.

9:15 243. Let's RAMP it up: Chemical safety management for high school laboratories. **K.J. Humphrey**

10:00 Coffee Break.

10:30 244. STEM students' perspectives, experiences, and expectations pertaining to genAI. **C. Sells**

11:15 245. Integrating ChatGPT in the chemistry classroom. **A. Iyer**, C. Zavacki

New Instrumentation, Trends, and Methods in Mass Spectrometry

T. Solouki, *Organizer, Presiding*

Lone Star 104

8:00 Introductory Remarks.

8:05 246. Protein footprinting by water photolysis. **K.K. Murray**, O. Ogundairo

8:35 247. Advancing the glyco toolbox: developing new sensitive MS-based methods to characterize glycan and glycopeptide isomers. **Y. Mechref**

9:05 248. Multi-omic analysis of Ebola infection. **B. Russell**, L. Palmer, T. Romsdahl, J. Linares

9:35 Intermission.

9:45 249. Novel approaches for physiologically relevant structural proteomics studies. P.K. Singh, L. Perez, S. Pardo, S.T. Weintraub, Q. Shi, **O. Klykov**

10:15 250. Improving ion activation on a Fourier transform ion mobility (FT-IM) Orbitrap mass spectrometer using a quadrupole ion guide. **K. Evans**, R. Schrader, C. Lantz, D.H. Russell

10:35 251. Leveraging protein unfolding and refolding dynamics to explore UV and IR laser ablation properties for native mass spectrometry imaging. **N. Feizi**, K.O. Hayes, B.C. Egbejiogu, K.B. Hines, K.K. Murray, T. Solouki

10:55 252. *i*prm-PASEF: An integrated workflow for the analysis and interpretation of spatial on-tissue tandem mass spectrometry of lipids. N. Tao, B. Heijs, S. Deininger, N. Kessler, A. Fuetterer, A. Behrens, C. Henkel, N. Smit, S. Ramachandran, **A. Eshghi**, K. Stumpo

11:25 Concluding Remarks.

Small Molecule Modulators of Cellular Function - Biology

T. Mitchell, D. Romo, *Organizers*
M. E. Abbasov, *Presiding*

Texas 115

8:00 253. Precision chemistry and activity-based proteomics for posttranslational control of protein function. **M.E. Abbasov**

8:30 254. Phenotypic drug discovery rejuvenated with new technologies for target identification. **D. Nijhawan**, J.K. De Brabander, J. Ready, T. Qin

9:00 255. Stereoisomeric probe sets for ligand identification via chemical proteomics. **Y. Tao**, M. Schafroth, D. Ogasawara, J.G. Felber, Z. Zou, D. Remillard, E. Njomen, J. Remsberg, E. Vinogradova, M. Yokoyama, D. Schwefel, C. Ye, B. Melillo, X. Zhang, C. He, S.L. Schreiber, B.F. Cravatt

9:30 Coffee Break.

10:00 256. Targeting bacterial virulence through two-component system signaling. **E.E. Carlson**

10:30 257. Dual leucine zipper kinase (DLK) inhibitors for the treatment of chemotherapy-induced peripheral neuropathy (CIPN). **g. liu**

11:00 258. Fully-functionalized natural products to expand the ligandable proteome. **C.M. Chaheine**

11:30 259. Pharmacophore-directed retrosynthesis applied to the selective TRPM7 ion channel inhibitor waixenicin A. **B. Gong**, M.R. Parris, S.A. Kiledal, S. Suzuki, A. Fleig, F.D. Horgen, D. Romo

11:45 260. Pharmacophore-directed retrosynthesis applied to the synthesis of curromycin a employing designed alkynyl proteomic probe intermediates. **C. Song**, M. Schwartz, C. Chaheine, S. Ranganathan, S. Sieber, J. Taube, D. Romo

Targeting the Tumor Microenvironment

K. G. Pinney, *Organizer, Presiding*
M. L. Trawick, *Presiding*

Texas 114

8:00 261. Multimodal imaging to evaluate tumor oxygenation, vasculature and vascular disruption for drug development. H.I. Wanniarachchi, K. Hamal, C. Pavlich, K.G. Pinney, M.L. Trawick, L. Liu, **R.P. Mason**

8:30 262. Targeting phosphatidylserine in the tumor microenvironment. **R.A. Brekken**

9:00 263. Repurposing cytotoxic chemotherapeutics as immune adjuvants to improve cancer treatment. **A. Risinger**, C. Fermaintt, L. Takahashi-Ruiz

9:30 264. Development of chemical reactions to advance drug discovery. **U.K. Tambar**

10:00 Coffee Break.

10:30 265. Caffeic acid phenethyl amide (CAPA) and analogues active against neuroblastoma. **S.M. Kerwin**

11:00 266. Small molecule activators of the integrated stress response for the treatment of leukemia. **J. Ready**

11:30 267. Betabody drug conjugates (BDCs) and antibody drug conjugates (ADCs) targeting phosphatidylserine (PS) in the tumor microenvironment with potent antimitotic/vascular disrupting agents. **M.L. Trawick**, R.A. Brekken, K.G. Pinney

Undergraduate Symposium

J. R. Ingle, *Organizer, Presiding*

Ranger 106/107

8:00 Introductory Remarks.

8:05 268. Targeting aberrant protein phase separation in human disease. **C.F. Knox**, O.L. Kipp, J. Nepogodin, L.R. English, S. Whitten

8:20 269. Novel cell death independent mechanism of acute anthracycline exposure in human cardiac fibroblasts. **K. Sadaka**

8:35 OPEN 270. MOVED to Sunday poster session P007 - Synthesis of chloropyridinol derivatives as possible histone deacetylase inhibitors (HDACi). **D. Abbott**, H. Shin, P. Pyenta

8:50 271. Pharmacophore-directed retrosynthesis applied to ophiobolin A: Potential cancer stem cell selective agent. **A. Hills**, J. Aroujo, H. Parker, J. Taube, D. Romo

9:05 Intermission.

9:10 272. Synthesis of Methotrexate loaded Poly L-lactic acid combined with a hydrogel for treatment of Rheumatoid Arthritis. **A. Khodair**

9:25 273. Rapid detergent solution phase separation driven formation of 2D nanosheets from membrane proteins and block copolymers. **K. Kimball**, R.J. Vogler, D. Bujanos, M. Kumar, B.D. Freeman

9:40 274. Tuning the phase separation properties of detergents for the crystallization of membrane proteins and block copolymers. **D.D. Bujanos**, R.J. Vogler, K. Kimball, B.D. Freeman, M. Kumar

9:55 275. Characterization of genes essential for hydrocarbon degradation by *Pseudomonas aeruginosa*. **T.A. Nguyen**, N. Del Campo, A. Rame, J.E. Dannatt, W. Cody

10:10 Coffee Break.

10:25 Introductory Remarks.

10:30 276. SPIDRR technique for measuring microcanonical rate constants of transition metal-mediated reactions. **W. Smith**, D.J. Bellert

10:45 277. Toward magnetic 2D lanthanide-based materials. **R. O'Shea**, A.B. Altman

11:00 278. Understanding linear scaling relations based on energy decomposition analysis. **J.D. DiCenso**, C. Lander, Z. Pei, T. Le, K. Gunasooriya, B. Wang, Y. Mao, Y. Shao

11:15 279. Characterizing surfactants and adsorbed asphaltene mimics in crude oil using self assembled monolayers. **O. Guzmán**, I. Guzmán, R.S. Thompson

11:30 280. Adsorption of complex molecules on SAMs to model crude oil mixtures: A quartz crystal microbalance (QCM) method development study. **I. Guzmán**, O. Guzmán, R.S. Thompson

11:45 281. Hybrid conferences: Attendee demographics and carbon footprint consequences. **B.S. Dawson**, R.J. Vogler, M. Gilb, H. Oh, M. Kumar

Stone Symposium: Unusual Structure, Reactivity, and Properties of Inorganic Species

C. Martin, S. Yruegas, *Organizers, Presiding*

Texas 113

8:45 Opening Remarks.

9:00 282. Building polynuclear clusters one metal atom at a time. M. Osei, H. Xu, N. La, A. Valles, Y. Moon, **R. Hernandez Sanchez**

9:25 283. Atomically precise metal cluster chemistry with stibine-based ligands. **A. Das**

9:50 284. Mechanistic studies of C-H activation in (PBP)Ir Complexes. V.T. Nguyen, R.N. Sladek, N. Bhuvanesh, J. Zhou, **O. Ozerov**

10:15 Coffee Break.

10:35 285. Organometallic reactivity modulated by dynamic coordination of a phosphine 1-azaallyl ligand. **J.M. Blacquiere**

11:15 286. Ligand flexibility and reactivity with tetrapodal metal complexes. J.M. Moore, H. Cho, **A.R. Fout**

11:40 287. Binary organometallics of PF_3 and CO in heterogenous systems – applied process development. **A.E. Carpenter**, B. Syring

MONDAY AFTERNOON

Bioinorganic Chemistry

P. J. Farmer, *Organizer, Presiding*

Texas 114

1:00 288. Interrogating nitrite reduction intermediates with a non-heme iron complex. **J. Moore**, A. Fout

1:30 289. Fluorescent protein based Zn2+ sensors for tracking labile Zn2+ in aerobically and anaerobically grown Escherichia coli. **H. Nguyen**, U. Huynh, M.L. Zastrow

2:00 290. *Engineering anaerobic FRET sensor for the detection of zinc ions in live cells*. **O. David**

2:30 291. Carboxylate-rich cobalt(II) complexes as phosphoesterase mimics in aqueous media. **G.T. Musie**

3:00 Coffee Break.

3:30 292. Synthesis and Characterization of Bismuth Nanoparticles as Imaging Contrast Agents. **A. Martino**, F. Mangano, B. Fallon, E.P. Greene, N. Mathuria, R.C. Willson, C.S. Filgueira

4:00 293. Proton-coupled electron transfer at a mis-metalated zinc site detected with protein charge ladders. **M. Gonzalez**, M.J. Guberman-Pfeffer, J. Koone, C.M. Dashnaw, T.J. Lato, B.F. Shaw

Computational and Theoretical Chemistry

K. L. Shuford, *Organizer, Presiding*

Texas 116

1:00 294. Unraveling the transport mechanism in fluoride ion channel. K. Mills, **H. Torabifard**

1:30 295. Application of AI in drug discovery. **G. Sharma**

1:50 296. SmartCADD: AI-QM Empowered Drug Discovery Platform with Explainability.. **A. Mahamada Kalapuwage**, E. Laird, C. Clark, E. Kraka

2:10 297. Using multiscale simulation to understand the impact of substituents modification in photo-isomerization of photostatins. **a. bakhtiiari**, R. Liang

2:30 298. Determination of the mechanism of controlled drug release from azobenzene-containing phosphatidylcholine liposomes using molecular dynamics simulations. **H. Mohammed Nazar**, K.A. Alberto, Z. Qin, P.A. Slesinger, S.O. Nielsen

2:50 Coffee Break.

3:20 299. Generating molecules with specific boiling points and melting points. **S.A. Alexander**

3:40 300. DFT study on iridium-catalyzed activation and silylation of inert γ-sp^3-C–H. **Y. Fan**

4:00 301. Conversion of biomass lignin derivatives into aromatic hydrocarbons: A quantum chemical study. **b. bangaru**

4:20 302. Reactivity of methyl diruthenium complexes with CO, Bipyridine and DPPM ligands. **S. Handunneththige**, X. Yang, R. Downey, R.M. Chin, M.B. Hall

4:40 303. QM/MM computations of active sites in hemoproteins. **M. Freindorf**, E. Kraka

Materials and Interfaces

Z. Zhang, *Organizer, Presiding*

Texas 118

1:00 304. Selective deposition three ways: Chemical bath deposition of metal sulfides on organic substrates. **A.V. Walker**

1:30 305. Non-contact thermometer for measuring surface temperature of photothermal catalysts using near-infrared blackbody radiation spectrum. **J. Bao**, M. Chirom, C. Qin, A. Lim, S. Baldelli, F. Robles Hernandez, D. Liu, V. Hadjiev, X. Shan, S.M. Louie, F. Lin

2:00 306. Terahertz time-domain spectrosocpy of quantum materials. **D. Hilton**

2:30 307. Role of Surface/Interface Phenomena in Antibacterial Action of Nano- and Microscale Zinc Oxide, Gallium Oxide, and Gallium Hydroxide. **Y. Strzhemechny**

3:00 Coffee Break.

3:30 308. Diatom Photonic Crystals for Chemical and Biological Sensing. **A. Wang**

4:00 309. Synthesis, Characterization, and Application of 2D Inorganic/Polymer Heterostructures. **y. zhu**, J. Lou

4:30 310. Engineering atomically thin semiconductors with moiré ferroelectricity. **D. KIM**, Y. Miyahara, X. Li

Molecular Imaging and Reporter Strategies

R. P. Mason, *Organizer, Presiding*

Ranger 106/107

1:00 Ralph Mason.

1:05 311. Precision imaging. **M.G. Pomper**

1:35 312. Glycloprotein-targeted radionuclide theranostic pair for CRC. **H. Manning**, R. Ta, A. Yamaguchi, R. Coll, K. McBride, S. Chauhan

2:05 313. Renal clearable nanoprobes for biomedical imaging. **J. Zheng**

2:35 314. Development of small molecule dyes and peptide-based contrast agents detectable using optoacoustic imaging. **L. McNally**

3:05 Coffee break.

3:30 315. 1,2-Dioxetanes for chemiluminescence imaging in cells and mammals. **A.R. Lippert**

4:00 316. Development of synthetic strategies to access fluorophores for biomedical research. **S.M. Usama**

4:30 317. Fluorescent sensors for imaging insulin secretion in vitro and in vivo. J. Gu, H. Zhang, **W. Li**

New Instrumentation, Trends, and Methods in Mass Spectrometry

T. Solouki, *Organizer, Presiding*

Lone Star 104

1:00 Introductory Remarks.

1:05 318. Proteome dynamics using metabolic labeling with deuterated water and LC-MS. **R.G. Sadygov**

1:35 319. Chemical tools for signature ion tracking in tandem MS: Applications to proteolytic and lipid modifications. **S.M. Chowdhury**, Z. Fang

2:05 320. An Iintegrated native ESI-MS approach for thermodynamic analysis of protein complex-ligand binding reactions. **D.H. Russell**

2:35 Intermission.

2:45 321. Mild and efficient Cu-catalyzed coupling reactions enabled by in situ electrolytically generated Cu cations in nanoelectrospray. **A. Sengupta**, D. Gunasekera, S. Xu, X. Yan

3:05 322. Determining thermodynamics of protein-lipid interactions using native mass spectrometry. **S. Kumar**, A. Laganowsky

3:25 323. Comparing the stability and strength of protein-ligand complexes in positive- and negative-ion mode native-like mass spectrometry. **M.G. Bannon**, M.S. Cordes, A.M. Cupples, E.S. Gallagher

3:45 324. Untargeted single cell lipidomics using trapped ion mobility spectrometry. **B. Wang**, J. Kim, D. Mun, S. Meyer, A. Barsch, E. Forsberg, A. Pandey, S. Byeon

4:15 Concluding Remarks.

Small Molecule Modulators of Cellular Function - Synthesis

Cosponsored by ORGN

D. Romo, *Organizer*

T. Mitchell, *Organizer, Presiding*

Texas 115

1:00 325. Oxidopyrylium-Based (5 + 2) Cycloadditions: *Old Roads, New Pathways*. **T. Mitchell**

1:30 326. Mild, additive-free thioetherification via proton transfer dual ionization mechanism. **C.R. Zwick**

2:00 327. Optimization of novel inhibitors of mycolic acid synthesis as TB drug candidates. **J.M. Schomaker**, J. Kim, P. Bartolomeu-Halicki, K. Rohde

2:30 Coffee Break.

3:00 328. G9A Inhibition: Induction of fetal hemoglobin for the treatment of Sickle Cell Disease. **M. Zancanella**

3:30 329. Total synthesis of dragocins A–C via electrochemical cyclization. **N.J. Truax**, B. Smith, A. Pollatos, M. Meanwell, P. Bedekar, A. Garrido-Castro, P.S. Baran

4:00 330. Discovery of a potent, selective, and efficacious small molecule inhibitor of NNMT as a potential therapeutic for treating solid tumors. **K. Kong**

4:30 331. Pharmacophore-directed retrosynthesis applied to ophiobolin A: Total synthesis, derivatization, and biological studies. **J. Aroujo**, Y. Tao, A. Hills, H. Parker, S. Rangananthan, J. Taube, D. Romo

4:45 332. Pharmacophore-directed retrosynthesis applied to talaromynoid H: Synthesis of the tetracyclic core and further elaboration to increasingly complex targets. **A. Youman**, P. Junghans, D. Romo

Synthesis and Growth of Nano to Bulk Solids for Energy and Environmental Applications

J. Chan, R. T. Macaluso, *Organizers, Presiding*

Lone Star 103

1:00 Welcome.

1:15 333. Evaluating the respiratory health effects of novel nano-enabled composites relevant to military applications. **C.M. Sayes**

1:35 334. Exercising synthetic control over the structures and photoelectrochemical properties of metastable semiconductors. **P.A. Maggard**

1:55 335. Understanding and controlling structural phase transitions in sodium-ion battery materials. **J. Bocarsly**

2:15 336. Designing and Architecting Battery Electrode Materials Across Length Scales. **S. Banerjee**

2:35 337. Novel narrow-bandgap heteroanionic oxypnictide semiconducting Zintl phases for thermoelectric applications. **S. Baranets**

2:55 Coffee Break.

3:10 338. Nanostructured bimetallic oxides and hydroxides: Designing active, stable and accessible materials for batteries and water splitting. **C.P. Rhodes**

3:30 339. Design Of Fluoride-Ion Battery Insertion Anodes based On Stereochemically Active Lone Pairs. **S. Hariyani**, G. Agbeworvi, A. Pakhira, C. Weiland, C. Jaye, L. Ma, S. Banerjee

3:45 340. Synthesis and phase stability of praseodymium ternary intermetallics. **M. Copeland**, A. Dominguez-Montero, G. McCandless, K. Wei, B. Schundelmier, J. Chan

4:00 341. Synthesis and Characterization of a series of Pressurized Lanthanide Diiodides. **H. Jemison**, A.B. Altman

4:15 342. Factors influencing activity and stability of Ru-based oxygen evolution electrocatalysts. **Z. Naymik**, C.P. Rhodes

4:30 343. New Eu(II)-containing chalcogenides with high SHG activities: Syntheses, crystal structures, electronic structure calculations and physical properties. **S. Jana**, P.A. Maggard

High School Educators Symposium

M. C. De Mesa, *Organizer*
A. Chu, K. Moos, *Presiding*

Ranger 110

1:30 344. Everything moles. **J. Flint**

2:15 345. Enhancing understanding of complex concepts through station-style introductory activities in the high school chemistry classroom. **C. Alexander**

3:00 Coffee Break.

3:30 346. The students become the teacher: Activities to visualize chemistry. **K. Moos**

Mechanisms of Genomic Repair and Mutagenesis

Cosponsored by TOXI

M. A. Trakselis, *Organizer, Presiding*

Texas 117

1:30 347. APOBEC mutagenesis in cancer. **R. Harris**

2:00 348. Mechanism of Smc5/6-mediated protein sumoylation in genome maintenance. **X. Xue**, J. Fan, P. Gallegos, X. Zhu, J. Epps, K. Holland, S. Li, X. Zhao

2:30 349. Ablating Ku70 phosphorylation disrupts the repair of non-ligatable DNA double-strand break ends resulting in increased radiation-induced genomic instability and carcinogenesis. **A. Davis**

3:00 350. Oxidative stress results in the accumulation of DNA damage within alternative DNA structures resulting in aberrant mutagenic processing. **M. Zewail-Foote**, I.M. del Mundo, A.W. Klattenhoff, K. Vasquez

3:15 Break.

3:45 351. The role of RING-between-RING (RBR) ubiquitin E3 Ligases in DNA repair. **J. Leung**

4:15 352. Structural basis of DNA Polymerase Theta (PolQ) mediated error-prone DNA synthesis and DNA double-strand break repair. **Y. Gao**

4:45 353. Formation and repair mechanisms of DNA-Histone cross-links. **K. Yang**

Stone Symposium: Unusual Structure, Reactivity, and Properties of Inorganic Species

C. Martin, S. Yruegas, *Organizers, Presiding*

Texas 113

1:45 354. Pnictogen bonding in solution. **A.F. Cozzolino**

2:10 355. Intramolecularly capping chalcogen oxides with boron Lewis acids. **B. Murphy**, F.P. Gabbai

2:35 356. Design and coordination chemistry of new NNN-based pincer ligands incorporating heavy Group 16 elements as pendant soft Lewis acids. A.L. Amaya, L. Delgado Cordoba, M. Abbasichaleshtori, H. Arman, A.F. Cozzolino, **Z.J. Tonzetich**

3:00 Coffee Break.

3:20 357. CO extrusion from a Ni Phosphaethynolate: Characterization and mechanistic insights. **M.T. Figgins**, R.R. Thompson, D.C. Wannipurage, A. Renteria-Gomez, A. Gogoi, J.A. Telser, D.L. Tierney, O. Gutierrez, D. Powers

3:45 358. Normal ligand field, inverted ligand field or other: applicability of the ligand field model in compounds that display unusual bonding patterns. **J. Shearer**

MONDAY EVENING

Gooch-Stephens Award Lecture

D. J. Bellert, *Organizer, Presiding*

McLennan Hall

5:45 Introductory Comments.

6:00 359. Capturing the molecular level mechanics driving bulk chemical behaviors from catalysis to the spectral dynamics of interfacial water with cryogenic ion spectroscopy. **M.A. Johnson**

6:55 Gooch-Stephens Award.

POSTER SESSIONS and EXPO and GRADUATE FAIR and RECEPTION

Brazos Ballroom

7:00 - 9:00 pm

Biochemistry Poster Session

L. R. Marshall, *Organizer*

360. Computational modeling of "chemically ready" conformations for enzyme catalysis studies. **S. Ranasinghe**, R. Van, X. Pan, Y. Shao

361. Selective delivery of anticancer agent KGP18 by a plasmin-cleavable drug-linker construct in the pancreatic tumor microenvironment. **P. Tankoano**, K. Hamal, W. Ren, R. Francis, K.G. Pinney, M.L. Trawick

362. Investigations of redox-based post-translational modifications on *Arabidopsis thaliana* stearoyl-ACP-desaturase. **C. King**, P. Horn

363. Synthesis and application of activity-based probes with tetrazole reactive groups for labeling glycoside hydrolases in gut commensal bacteria.. **J. Russo**, A.T. Wright

364. Towards studies of PRODH enzyme dynamics using X-ray crystallography. **F. Akter**, D. P. Buckley, J. Tanner, J. Clinger

365. Translesion synthesis (TLS) polymerases Eta and Rev1 coordinate their activities for efficient lesion bypass and on noncanonical templates. **T.I. Punchipatabendi**, **S. Disha**, **J. Kaszubowski**, **H. Chu**, **M.A. Trakselis**

366. Specific little finger residues i.e. Pinky Trigger in Y family polymerases restrict downstream synthesis past lesion. **S. Disha**, J. Kaszubowski, T.I. Punchipatabendi, J. Pata, M.A. Trakselis

367. Development of a single particle CryoEM pipeline at Baylor University. **J. Koone**, D. Berti, B. Zechmann, J. Clinger

368. In-cell directed evolution of a ratiometric fluorescent biosensor for chloride. **S. Phelps**, J. Tutol, S. Dodani

369. Structural and biochemical characterization of Rad7-Rad16 in *Saccharomyces cerevisiae* nucleotide excision repair. **C. Hewa Bhashithage**, J. Min

370. Influence of intramolecular epistasis on catalytic promiscuity and enzyme specificity among protein homologs. **G. Owusu-Addo**, A. McMilla, D. Odokonyero, M. Zhu, K. Hull, D. Rom, M. Glasner

371. Investigation of replication restart pathways utilized to mitigate replisome decoupling in *Escherichia coli*. **S. Fernando**, **C. Agadagba**, M.A. Trakselis

372. Rescuing Lactoperoxidase Expression with CRISPR/Cas9 system and Antagomirs to Mitigate Lung Inflammation in smokers and COPD patients. **M.J. Santiago**, S. Chinnapaiyan, K. Panda, M. Rahman, S. Ghorai, H.J. Unwalla

373. Characterization of a non-NFK dioxygen product catalyzed by a bacterial putative TDO. **D.W. Valencia**, I. Shin, D. Wherritt, A. Liu

374. Analyzing energy transference in the γ Subunit of *Escherichia coli* ATP synthase through terminus extension. **E.T. Victor**, Y. Li, M. Stankus, A. Penny

375. Fluorescence quenching of human serum albumin by organochlorine pesticides. J. Luke, L. Hicks, A. Mishra, **R. Yadav**

376. Using circular dichroism to explore favored alpha helical stability in designe peptides. **E. Kingston**, **A. Malladi**, J.A. Hebda

377. Exploring the mechanosensitive behavior of PIEZO ion channels: A computational study on conformational dynamics. **O. Saibu**

378. Computational modeling of C-terminal loop of voltage-gated sodium channel 1.4 in humans and grasshopper mice. **E. Jones**, R. Van, A. Rowe, Y. Shao

379. Probing the metalation state dynamics of histone deacetylases. **L. Kimberly**, E.L. Que

380. Structural dynamics of PriB, a C-prenyltransferase. **O. Ogundele**, J. Clinger

381. Site-specific contacts that activate DNA unwinding by HROB/MCM8/9. **C. To**, C. Li, Y. Gao, M.A. Trakselis

382. Examining the energy transmission mediated by two loops in the γ subunit of *Eschericia coli* ATP Synthase. **A. Penny**, M. Stankus, E. Victor, Y. Li

383. Dynamics study of Ornithine Decarboxylase: Applications in structural biology. **K.P. Ezennubia**, J.C. Koone, J. Clinger

384. Interference of Kaempferol and its derivatives in amyloid beta-peptide aggregation: AFM and optical spectroscopic approaches. **B. Sengupta**, R. Friedfield

P001. Mechanism of the Rad34-Rad23-Rad33 in RNA Polymerase I-associated transcription-coupled nucleotide excision repair of yeast. **M. Dalpathadu**, L. Pham, K. Murakami, J-H. Min

P006. Structural and functional understanding of the eukaryotic Global Genome Nucleotide Excision Repair pathway. **T. Adeniran**, L. Pham, K. Murakami, J-H. Min

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Environmental Chemistry and Toxicology Poster Session

G. P. Cobb, C. M. Sayes, *Organizers*

385. Zero-valent iron nanoparticles differentially affect diverse bacterial species. **B.J. Carnathan**, M. Stevens, C.M. Sayes

386. Microgel composites using carbon nanotubes as flocculants for sustainable environmental applications. **M. Islam**, P. Otuokere, V. Robinson, Y. Gao

387. Utilizing rapid enzymatic activity model (REAM) to decipher potential toxicity mechanisms of herbicides- glyphosate and atrazine. **L.K. Vuu**, P.C. Obiako, C.M. Sayes

388. Synergistic optimization of microalgae Chlorella vulgaris carbon sequestration through photocatalytic utilization of ZnO nanoparticles. **L.P. Salmeron-Covarrubias**, K. Beluri, H. Sharifan

389. Effect of metal-organic framework(MOF) particle size on chromate removal from aqueous solutions. **o. Raji**

390. Receptor-ligand relationship of *Aedes aegypti* IR75D and hexanoic acid. **M. Chembars**, J. Pitts

391. Using ferrihydrite to capture inorganic arsenic from subrogate fertilizers. **R. Smith**, B. Perry, D. Toole, G.M. Chiarella

392. Capturing inorganic arsenic fron fertilizers by using goethite as a metal complexation technique. **B. Perry**, R. Smith, D. Toole, G.M. Chiarella

393. Optimization of chitin extraction using deep eutectic solvents. **S. Holdar**, D. Gibson II

394. Plant-based dyes as alternative fluorescents for microplastics under a microscope. **M. Cervantes**, K.L. Bryan, I. Nowowiejski, D. Gibson II

395. Microbial Biofilm Formation by *Bacillus thuringiensis* in treated wastewater from deep east Texas wastewater treatment plants. **O.O. Ogunlewe**, P. Baker, B. Sengupta

396. Selective removal of dyes from water using quality-downgraded fluorinated single-walled carbon nanotubes. **P.U. Otuokere**, M. Islam, V. Robinson, Y. Gao

397. *Withdrawn*

398. Chlorhexidine interaction with microcrystalline cellulose. **U. Joshi**, **M. Martinez**, J.D. Beatty

399. Determining the effect of atmospheric pollution on *Sphagnum* in north England peatlands. **A. Treadway**, L. Horton, A. Creevy, J. Clear

P005. Detection of Polycyclic Aromatic Hydrocarbons via Fluorescence Resonance Energy Transfer. **V. Salazar**, N. McDaniel, H. Fernando

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Organic Chemistry Poster Session

N. Matsumoto, *Organizer*

400. Chemical safety and security challenges in academic institutions in southern region of Somalia. **A.S. Mohamed**

401. Biocatalytic Aza-Michael addition of aromatic amines to enone using α-Amylase in water. **S. DUTT**

402. Design, Synthesis and Structure-Activity Relationship of CNS Penetrant Small Molecule ER-Beta Agonists for Glioblastoma (GBM) Therapies. S.F. McHardy, **A. Maciolek**, U. Pratap, S. Viswanadhapalli, M. Tidwell, K. Nieves-Merced, A. Brenner, R. Vadlamudi

403. Development of potent and selective YAP-1 inhibitors and degraders: Lead optimization and *in vitro* proof- of-concept studies. S.F. McHardy, **L. Barrera**, U. Saran, R. Amaradhi, P. Barrodia, S. Satpati, B. Singh, K. Rai

404. Synthetic strategies towards Fusicocane diterpenoids. **D. Henderson**, J.L. Wood

405. Coupling photocatalysis and substitution chemistry to expand and normalize redox-active halides. **M. Rathnayake**, J.D. Weaver

406. Total syntheses of erchinines a and b. **Y. Cho**, J.L. Wood

407. Investigation of Cobalt(II) complexes for photocatalyzed reactions under visible light irradiation. **S. Pal**, S. Pitre

408. Chemiluminescent 1,2-dioxetane for imaging of hypochlorous acid. **C. Griffin**

409. Mechanistic studies of the decomposition of 1,2-dioxetanes in aqueous conditions. **M. Castro**

410. Diazo Compounds and pH Control: Separating Sidechain and C-terminal Reactivity. **A. Omere**

411. Catalytic chemo-, regio-, and diastereoselective bromochlorination of (poly)unsaturated starting materials. **A.E. Lubaev**

412. Computer aided drug design and synthesis of voltage-gated sodium channel inhibitors. **C.B. DeVerter**, N.A. Clanton, D. Biscardi, D.E. Frantz

413. Synthesis of 1,2,3,5-Tetrasubstituted-1*H*-Indoles via a Domino Reaction Sequence. **S. MAJI**, K. Fobi, E. Ametsetor, R.A. Bunce

414. Convergent total synthesis of Aleutianamine. **J.P. Tuccinardi**, J.L. Wood

415. Copper ion specific chemiluminescent probe. **R. Osman**

416. Halogen-bonding photocatalysis using carbazole-based electron donor catalysts. **N. Shafiei**, T. Tasnim, S. Pitre

417. *Expanding the scope of SuFEx nucleophiles beyond amines and alcohols*. **A. Choudhury**, Q. Michaudel

418. Total synthesis of (-)-flueggeacosine C. L. Liu, **T. Olson**, J.L. Wood

419. Pharmacophore-directed retrosynthesis applied to colletotrichone A. **J. Yoder**, W. Ding, S. Sieber, D. Romo

420. Design and synthesis of proteolysis targeting chimeras (PROTACs) for tubulin degradation. **C. Borchardt**, K.G. Pinney

421. Design of a molecular motor based on a redox switchable aminoxyl ring. **C. Ou**, Y. Feng

422. Near-infrared chemiluminescent 1,2 Dioxetane probe for the detection of Copper (II) Ion. **G. Chen**

423. Photolytic access to spirodihydrofurans and chromenes from vinyldiazo ester cycloaddition with p-quinones. **S. Fremin**

424. Pharmacophore-directed retrosynthesis applied to Thia-Salarin C. **M. Parris**, E. Woods, R. Jourdain, H. Xue, D. Romo

425. Radical reactions with chiral acylammonium salts: Synthesis of functionalized delta-lactams through Giese-initiated organocascades. P.J. Sutter, **B. Walker**, K. Kasper, V. Kojasoy, D.J. Tantillo, D. Romo

426. Iridium-catalyzed enantioselective conjunctive cross-coupling of bis(alkenyl)boronates. **M. Tran**, J. Ready

427. Chemomechanical characterization of V2O5 single crystals via nanoindentation and in situ lithiation. **V.H. Balcorta**, R. Lee, R. Patel, S. Kotze, A. Maji, J. Ponis, C. Walker, G. Pharr, K. Xie, S. Banerjee, M. Pharr

428. Progress towards the total synthesis of nargenicin A1. **J. Olsen**

429. Synthetic studies for the development of an oxidative chiral resolution platform to access α-hydroxy carbonyl compounds. **W.A. Badmus**, M.E. Hinze

430. Palladium catalyzed rearrangement of 2-benzyloxyfurans into substituted butenolides. **J. Shah Gupta**

431. A vision-guided, high-throughput platform for liquid-liquid extraction screening. **S. Moor**, A. Sun

432. Deaminative C–C Cross Couplings Through 1,2-Dialkyldiazene Photosensitization and Nickel Catalysis. **M. Diaz**, D. Chattapadhyay, A. Aydogan, Q. Michaudel

433. Palladium-catalyzed borylative difunctionalization of alkenes. K.L. Hull, **H. Pham**, S. Bhatt, Y. Wang

434. Synthetic studies towards Atkamine. **C.F. Graf**, J.P. Tuccinardi, J.L. Wood

435. Pharmacophore-directed retrosynthesis applied to the immunomodulatory natural product aspertaichunol A. **T. Coburn**, D. Romo

436. Palladium-catalyzed cyanations of aryl imidazolylsulfonates with K4[Fe(CN)6]: A pragmatic approach to benzonitriles from phenols. **W.M. Palmer**, N. Wilson, D.E. Frantz, m. levorse, J. Coombs, J. Ganley, J. Albaneze-Walker

437. Directed sinthesis of Agelastatin A derivatives with potential activity toward glioblastoma. **T. Goulart**, J. Taube, D. Romo

438. Amino Acid-Ni(acac)$_2$ complex catalyzed domino Michael-Henry Reaction of 1,2-Cyclohexanedione with Nitroolefins. **M. Cain**, B. Ni

439. Merck Chemistry: Discovery and small molecule process research & development. **S. Dishman**

440. Progress towards the synthesis of verrillin. **P. Duc**, J.P. Tuccinardi, J.L. Wood

441. Total synthesis of fusicoccane diterpenoid natural products. **W. Bonnet**

442. Study on the formation of diazaborolidines from phenylboronic acid derivatives and 1,2-diamines. **R. Pathirana Hewage**, D.E. Gross

443. Computational study on the hydrolytic stability of heteroboroles.. **G. Ariyaratne**, D.E. Gross

444. Application of pharmacophore-directed retrosynthesis to the dichapetalins. **N. Matsumoto**, E. Woods, T. Coburn, S. Lin, D. Ilangasinghe, G. Ross, D. Gann, D. Romo

445. Zirconocene hydride-catalysed transaminative dual reduction of amides via steady state imine. **A. Raj**

446. Synthesis, In-vitro and In-silico Evaluation of Novel Pyrazolone Hybrids as Potential Anticancer Agents. **S. Dahal**, S. Murru, P. Anim Addo, A. Agu, A. Gholamian Moghaddam

447. De novo synthesis of the derivatives of WaixenicinA. **U. Boddu**

448. *Withdrawn*

449. Building up maximum strain energy in a conjugated macrocycle. **C.S. Lawrence**, M. Mirzaei, M. Mirzaei, R. Hernández Sánchez

450. Investigation of the Benzyl Esterification of *trans*-Arylcycloalkenes. **H. Keith**, T. Schoch, J.D. Weaver

451. Optimization of co-catalytic coupling of secondary alkyl chloride; the curious role of Lutidine. **A. Ethridge**, P. Sharma, R. Hanumanthu, J.D. Weaver

452. *Withdrawn*

453. *Withdrawn*

Polymeric Materials Science and Engineering Poster Session

R. Foudazi, *Organizer*

454. Metal-Induced hydrogel and selective antibacterial nanomaterial synthesis using hydrophilic polypeptides. **J. Cho**, W. Yang, L. Hanna, W. Dodson, Y. Qamar, H. Galmiche, L. Allain, J. Revere

455. *Withdrawn*

456. pH-responsive zwitterionic material for bioremediation and biomedical applications. **M. Mukut**

457. Towards optimizing performance of foam-templated porous hydrogels. **S. Onyembe**, R. Foudazi

458. Detection of cortisol in human sweat using nitrogen-doped graphene quantum dots coated in a polyethylyne oxide/polyaniline blend film. **C. Sanchez**, D. De Leon, A. James, N. Barbosa, A. Jalal, A. Mikhoyan, J. Parson, K. Lozano, V. Padilla

459. Sample Preparation and Analysis of Polyurethane Rigid Foams via Scanning Electron Microscopy. **T. Le**

460. Graphitic carbon nitride catalyze azo bond reduction by hydrazine under visible light. **G. Ollordaa**, L. Yingchun

461. Lyotropic liquid crystal-templated membranes from self-assembly of amphiphilic block copolymers. **S. Tabatabaei**, R. Foudazi

462. Thermally reversible and NIR light-sensitive agarose hydrogels for controlled drug release. **S. Bhuiyan**, T. Betancourt

463. Lipid metal-organic framework hollow colloidosomes. **J. Podliska**, R. Ravanfar

464. Morphology and crystallinity of gel polymer electrolytes containing Poly(ethylene oxide). **F. Naderi Samani**, R. Foudazi

465. Development of porous methylcellulose and cellulose acetate based fibers for applications in antibacterial wound dressing. **A. James**, D. Philips, E. Varughese, M. Uddin

466. Organic pollutant adsorption on synthesized metal-organic frameworks: Computational investigation. **M. Mapula**, S. Lin

TUESDAY MORNING

Chemical Biology

A. T. Wright, *Presiding*

Texas 117

8:00 467. Lighting up cellular chloride transport. **J. Tutol**, W. Ong, H.C. Kam, S. Phelps, W. Peng, H. Goenawan, S. Dodani

8:30 468. Development of a fluorescent lateral flow test for the detection of the obesity biomarker leptin. **M. Ortiz**, K. Kourentzi, R.C. Willson, M. Rito-Palomares, M. González-González

9:00 469. Digital light processing (DLP) fluorescence microscopy for 3D microprinting and single cell photoactivation. **A.R. Lippert**

9:30 470. Unraveling the molecular interactions of trehalose glycolipds with bioorthogonal chemical approaches. **J.A. Buonomo**

10:00 Coffee Break.

10:30 471. Leveraging catalytically promiscuous enzymes to probe the basis for enzyme specificity and epistasis. D. Truong, A.W. McMillan, D. Odokonyero, R. Dharmatti, D. Suriadinata, R. Skouby, J. Huddleston, S. Fults, C. Davila, R. Bayana, M. Zhu, K. Hull, D. Romo, F.M. Raushel, **M. Glasner**

11:00 472. Biomolecular condensates promote cancer signaling. **J. Guan**

11:30 473. Responsive protein switches to probe cell and tissue behavior. **B. Belardi**

Computational and Theoretical Chemistry

K. L. Shuford, *Organizer*
U. De Alwis, *Presiding*

Texas 116

8:00 474. Enhancing material development through multiscale molecular modeling: case studies in viscosity prediction and polymer optimization with Simcenter Culgi. J. Lopez, T. Sweere, **R. Aglave**, **C. Tourani**

8:20 475. Simulations of core-hole induced attosecond electron dynamics. **L. Kurkowski**, T. Hua, K. Lopata

8:40 476. Hybrid and mixed basis set strategies for XPS calculations of small water clusters. **A. Delgado**, D. Matthews

9:00 477. Simulating fluorescence for mesoscale molecular aggregates. **T. Gera**, A.J. Hartzell, D. Raccah

9:20 478. LModeA Extension to Periodic System: The gateway for a quantitative characterization of normal modes in neutron scattering and terahertz spectroscopy. **F. Bodo**, A. Erba, E. Kraka

9:40 479. Computer-aided design of 2D transition metal-based alloy compounds for sustainable energy applications. **U. De Alwis**, V. Choutipalli, K.L. Shuford

10:00 Coffee Break.

10:20 480. Mechanistic insights into S-depalmitolyse activity of Cln5 protein linked to neurodegeneration and Batten disease: A QM/MM study. **Y. DANGAT**

10:40 481. *Withdrawn*

11:00 482. Signatures of hydrogen bonding in soft X-ray spectroscopy. **A. Yousaf**

11:20 483. Predicting halogen bond properties through machine learning. **D. Devore**, K.L. Shuford

11:40 484. Noncovalent interactions in apo-myoglobin proteins revealed through local vibrational mode theory. **J. Antonio**, E. Kraka

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Electrocatalysis: Molecular and Material Approaches to Electrified Chemical Processes

D. Boucher, *Organizer, Presiding*

Lone Star 104

8:00 485. Quantum-mechanical molecular dynamics simulations and analysis of graphene-catalyzed oxygen reduction reactions. **R.A. Grove**, C.F. Negre, M.E. Wall, I. Matanovic, J.D. Finkelstein, A.M. Niklasson

8:30 486. Metal-free C–H amination via bidirectional proton-coupled electron transfer (PCET) at anodically generated iodanyl radical intermediates. **P. Thai**, B.L. Frey, L.H. Patel, R. Lalisse, Z. Song, R. Carmieli, O. Gutierrez, D. Powers

9:00 487. Symmetry driven silicon-molecule interfacial design for photoelectrochemical hydrogen generation. **C.D. Hallock**, J. Brinker, M.J. Rose

9:30 488. Interfacing high-throughput electrosynthesis and mass spectrometric analysis of azines. **E.A. Hirtzel**, K.M. Kulesa, X. Yan, L.A. Baker

10:00 Coffee Break.

10:30 489. Deciphering the Role of Aromatic Cations in Electrochemical CO_2 Reduction: Interfacial Ion Assembly Governs Reaction Pathways. **W. Guo**, B. Liu, S.R. Anderson, S.G. Johnstone, M.A. Gebbie

11:00 490. Confocal Raman microscopy in the study of electrode-supported catalyst and thin films. **C.L. Korzeniewski**

11:30 491. Mapping the local electrocatalytic activity and selectivity via hybrid SECM-SECCM. **C. Ryu**, **H. Ren**

F-elements: Structure and Applications Part 1

A. E. Gorden, *Organizer*
J. Ducilon, *Presiding*

Texas 113

8:00 Introductory Remarks.

8:10 492. Discovery and strategic synthesis of *f*-element quantum intermetallics. **J. Chan**

8:40 493. Fostering new aspects of organolanthanide pincer chemistry: Applications for lanthanide luminescent complexes. **S. Chowdhury**, A.B. Altman, A.R. Fout

9:00 494. Synthesis and characterization of *d-f* heterometallic clusters. **B.G. Barnes**, A. Briseño, C. Windorff

9:20 495. Engendering orbital specific control in lanthanide complexes. **A.B. Altman**, S. Chowdhury, P. Reuel, H. Jemison, R. O'Shea

9:50 Coffee.

10:30 496. Unexpected products from lanthanide coordination reactions: Consequences and solutions. **E. Fatila**

11:00 497. Pursuit of organouranium nitride clusters and preparation of a transuranium facility. **C.J. Windorff**

11:30 498. F- element complexes with functionalized salophen-type mixed donor ligands. **A.E. Gorden**

Materials and Interfaces

Z. Zhang, *Organizer, Presiding*

Texas 118

8:00 499. Examing technologically relevant materials via interface engineering. **A. Yost**

8:30 500. Digital atomically precise lithography for direct write and nanoImprint mask writing. **J.N. Randall**, J.H. Owen, J.B. Ballard, U. Fuchs

9:00 501. Enhanced operational stability of perovskite light-emitting devices through differential ion motion. **J. Slinker**

9:30 502. Element-sensitive characterization of high-entropy oxide perovskite thin films. **A. Farhan**

10:00 Coffee break.

10:30 503. Fundamental investigation of the interfacial properties of CoCrFeNi high entropy alloy. F.A. McKay, A.N. Okafor, D.P. Young, P. Sprunger, **Y. Xu**

11:00 504. Advanced surface engineering coating technologies for industry applications. **J. Lin**, V. Zorbas Poenitzsch

11:30 505. Phase transition and melting of oxide via plasmonic heating. **Z. Zhang**

Metalloenzyme Design

I. V. Korendovych, *Organizer, Presiding*

Texas 114

8:00 506. Hybrid metalloproteins for photocatalytic CO2 and proton reduction. **G. Ghirlanda**, A. Banerjee, M. Rahman

8:40 507. Copper-catalyzed cross coupling approaches to selective PTM modifications. **Z.T. Ball**

9:20 508. Achieving catalytic hydroxylation of methane through manipulation of P450BM3 biotransformations with decoy molecules. **O. Shoji**

10:00 Coffee break.

10:30 509. Spectroscopic evaluation of the stability of the New Dehli metallo-β-lactamase (NDM-1).. S. Pennock, **G.A. Caputo**

11:00 510. Designing catalytic amyloids to function as highly efficient metalloenzymes. **L.R. Marshall**, I.V. Korendovych

11:30 511. How does modulation of the primary, secondary, and outer-sphere interactions in de novo-designed artificial Cu proteins (ArCuPs) affect their electron transfer and C-H peroxidation functionality?. **S. Chakraborty**, D. Prakash, S. Mitra, S. Sony

Novel Approaches to Drug Delivery

R. R. Kane, *Organizer*
J. J. Gassensmith, *Organizer, Presiding*

Texas 115

8:00 512. Guns, germs, and MOFs (and COFs!). **J.J. Gassensmith**

8:30 513. Developing drug delivery systems for chronic infectious diseases. **h. Smyth**

9:00 514. Image-guided drug delivery using radiation therapy: Strategic trade-offs in chemical design. **M. Miller**

9:30 515. Engineering cell based drug delivery with chemically self-assembled nanorings. **C.R. Wagner**

10:00 Coffee Break.

10:30 516. Biomaterial for *in situ* manufacturing and delivery of CAR t-cells. **Y. Brudno**

11:00 517. Bioengineering cell-based therapeutics. **O. Veiseh**

11:30 518. Amphiphilic polycaprolactone diblock copolymers for drug delivery of anticancer drugs. H. Polara, M.C. Biewer, **M. Stefan**

12:00 519. Lectin drug conjugates targeting high mannose N-glycans. S. Kurhade, **M.P. Farrell**

Polymers and Sustainability Challenges 1

R. Foudazi, *Organizer, Presiding*

Ranger 106/107

8:00 Introductory Remarks.

8:05 520. Stochastic model regression and analysis of repeat unit sequencing of Poly(lactide-co-glycolide). **N.A. Lynd**

8:30 521. Sugars as a platform for functional materials. **S.L. Kristufek**

8:55 522. Self-contained cost effective plastic recycling facilities:. **R.K. Vaidyanathan**, S.P. Chaudhari, C. Switzer, A. Maheshwari, F.D. Blum

9:20 523. Dynamic covalent polymer networks: Stereochemically controlled shape morphing. **S.A. Sukhishvili**

9:45 Intermission.

10:15 524. Sustainability through microarchitecture. **W. Voit**

10:40 525. Engineering and chemistry considerations to enable a circular economy of polymers. **D.S. Germack**

11:05 526. Valorization of cottonseed byproducts for bioplastic (biocomposite, biofilm) applications. **Z. He**, S. Nam, H.N. Cheng, A. Biswas

11:30 527. Carpets and bottle parts: A match made in the lab. **F.D. Blum**, R.Y. Azarfam, A. Maheshwari, L.A. Kamran, A.S. Nayar, S.P. Chaudhari, C. Switzer, J.C. Hanan, R.K. Vaidyanathan

Assessments for Learning and Engaging with Students

A. Sra, M. Stover, *Organizers, Presiding*

Ranger 110

8:30 Welcome and Brief Introduction.

8:35 528. Assessments: Time for a change. **A. Sra**

9:05 529. Using particulate representations to assess students in introductory chemistry courses. **S.G. Prilliman**

9:30 530. Microcredentials in the co-curricular undergraduate experience. **R.T. Macaluso**

10:00 Coffee Break.

10:30 531. Contextualized Chemistry Learning Materials and the Impacts on General Chemistry Students' Learning Outcomes. **I. Sristy**, Y. Vasquez, J. Mutambuki

10:55 532. Introducing activities to enhance literature reading skills in biochemistry. **M. Kopecki-Fjetland**

11:25 533. Examining analytical chemistry student interpretation of IR spectra. **M. Atkinson**

Atmospheric Chemistry

Y. Li, R. J. Sheesley, *Organizers, Presiding*

Lone Star 103

10:30 534. Modeling atmospheric decamethylcyclopentasiloxane (D5) concentrations in Houston using the community multiscale air quality model. **H. Yim**, A. Dodero, Y. Zhang, Q. Ying

10:45 535. Atmospheric oxidation capacity and air quality trends in Texas due to long-term climate and anthropogenic emission scenarios. **A. Gonzalez**, Q. Ying

11:00 536. Comparison of mobile and stationary measurement of formaldehyde by Picarro's G2307 and Aero-Laser's AL4021. **P. Sharma**, S.L. Alvarez, S. Yoon, J.H. Flynn, S. Usenko, R.J. Sheesley

11:15 537. Quantification of atmospheric alkanes and polycyclic aromatic hydrocarbons (PAHS) in the arctic region. **P.K. Verma**, T. Matthews, R.J. Sheesley

11:30 538. Role of Aerosol Chemical and Physical Properties in Cloud Formation. **S.D. Brooks**, Z. Lei, T. Pena, S.A. Thompson, B. Chen, B.H. Matthews, A. Rapp, C.J. Nowotarski

11:45 539. Identification and quantification of Per- and Polyfluoroalkyl Substances (PFAS) using Vocus 2R Chemical Ionization Mass Spectrometer (CIMS) with NO^+ Reagent Ion. **S. Gagan**, M. Olin, S. Niu, A. Dodero, M.J. Davern, G.V. West, B.J. Turpin, J. Surratt, Y. Zhang

TUESDAY AFTERNOON

Atmospheric Chemistry

Y. Li, R. J. Sheesley, *Organizers, Presiding*

Lone Star 103

1:00 540. Spectroscopy and Photochemistry of Wildfire Brown Carbon. **A.W. Harrison**

1:15 541. Identification of biomass burning smoke influence using aerosol optical properties and hydrogen cyanide in Fort Worth, Texas. **J. Poudel**, L. Senkbeil, M. Mehra, S. Yoon, J.H. Flynn, T.I. Yacovitch, C. Daube, E. Fortner, S. Usenko, R.J. Sheesley

1:30 542. Identification and characterization of biomass burning smoke in Houston, TX: Insights from the BC2 Aerosol Optical Network. **M.T. Ramirez**, L. Senkbeil, M. Mehra, S. Shrestha, J. Flynn, R.J. Sheesley, S. Usenko

1:45 543. Assessing air quality benefits of better managing natural and working lands in California. **S.M. Lindsey**, Y. Li

2:00 544. Investigating climate impacts of reducing methane emissions from U.S. landfills. **A. Folorunsho**, Y. Li

2:15 545. Estimating surface methane concentrations across the U.S. using Artificial Neural Network (ANN) and their application for tracking landfill emissions. **M. Bade**

2:30 Discussion.

Battery Materials, Chemistries, and Strategies

Cosponsored by ENFL

J. Larson, *Organizer, Presiding*

Texas 116

1:00 546. Unravelling the fundamental issues for improving lithium metal anodes based on three-dimensional nanostructured carbon hosts. **J. Li**, S. Rajendran, a. sekar

1:28 547. Structural, Electronic, and Chemical Evolution at Interfaces: Impact on Meso- and Macroscopic Properties. **P. Balbuena**, S.P. Beltran, D. Kuai, F. Ospina-Acevedo

1:56 548. Materials design strategies for elastic ceramic-based solid state electrolytes in advancing performance in lithium metal batteries. S. Bashir, **J.L. Liu**

2:24 Coffee Break.

2:54 549. Rapid synthesis and surface engineering of oxide solid electrolytes for lithium-metal batteries. **H. Khani**

3:18 550. Analysis and simulation of lithium-metal anodes of rechargeable batteries for vehicular transport. **J.M. Seminario**

3:42 551. Chemical and physical activation methods to develop highly porous materials for Li-S Batteries. **N. Siraj**, A. Oyebade, I. Denmark

4:06 552. Biomaterials for lithium-ion batteries. **H. Ardebili**, **N. Khiabani**, Q. Fu, M. Yuan, S. Adaryan, J. Fan, K. Bourland, M. Kammoun, D.F. Rodrigues

4:30 553. Regulating crystallization at dynamic electrochemical interfaces in battery electrodes. **K.J. Zheng**

Chemical Biology

A. T. Wright, *Presiding*

Texas 117

1:00 554. DNA-based tools for chemical and biological sensing. **D. Samanta**

1:30 555. Ubiquitin azapeptide esters as next-generation activity-based probes for mapping cysteine enzyme activities in the ubiquitin-proteasome pathway. **W. Liu**

2:00 556. Broadening the ligandable proteome using tyrosine-reactive electrophiles. D.M. Leace, H.M. Budaraju, N. Reddy, **K. Hsu**

2:30 557. Aza-enediynes: From DNA cleavage agents to covalent probes for protein kinases. **S.M. Kerwin**

3:00 Coffee Break.

3:30 558. Using chemical biology tools to study amino-acid based (proton-coupled) electron transfer. **C. Tommos**

4:00 559. Crosslinking technologies for studying viral and allergenic protein complexes. **S.M. Chowdhury**, A. Talukder, S. Cornelius

4:30 560. Photocrosslinking sugars for glycoconjugate interaction discovery. A. Ghorashi, R. Konada, **J.J. Kohler**

Engineering of Biochemistry for Enhanced or Novel Activity

J. Clinger, I. V. Korendovych, *Presiding*

Texas 115

1:00 561. Incorporation of synthetic metal complexes into heme acquisition protein HasA for selective photosterilisation of pseudomonas aeruginosa. **O. Shoji**

1:40 562. Protein engineering to combat pathogens. **B. Berger**

2:20 563. Ancestral proteins as scaffolds for enzyme engineering and evolution. **J. Sanchez-Ruiz**

3:00 coffee break.

3:30 564. Stimuli-responsive materials for wound healing and drug delivery. **O. Makhlynets**

4:00 565. NMR-guided directed evolution. **I.V. Korendovych**

4:30 566. Development of biologically equivalent simulant for forensic applications. **J.L. Liu**, E. Rancourt, M. Sandoval, S. Bashir

F-elements: Structure and Applications

A. E. Gorden, *Organizer*

J. Ducilon, *Presiding*

Texas 113

1:00 Introduction and Discussion.

1:10 567. Design Principles for Insertion Electrodes and Solid Electrolytes of Anion Batteries. **S. Banerjee**

1:40 568. Tuning the Ru_3Sn_7 structure type with samarium. **K. Brown**, B. Schundelmier, K. Wei, G. McCandless, J. Chan

2:00 569. Promoting covalent bonding in lanthanides: Reduced lanthanide-aluminum heterobimetallic complexes. **P. Reuel**, A.B. Altman

2:20 570. New developments in actinide organometallic chemistry. **J.L. Kiplinger**

2:50 Coffee.

3:30 571. Predicting structure type and properties in the $Ln_2M_3X_5$ family. **M. Plata**, S. Smith, J. Chan

3:50 572. Enabling wide-gamut human-centric display lighting. **S. Hariyani**, X. Xing, M. Amachraa, J. Bao, S. Ong, J. Brgoch

4:20 573. Coordination network of trivalent plutonium with bromoterephthalate and glutarate entities. **R.A. Zehnder**

Materials and Interfaces

J. Larson, Z. Zhang, *Organizers, Presiding*

Texas 118

1:00 574. Theory-guided design of "golden triangle metal-inorganic frameworks" (GT-MIFs) with chemisorption-active macrometallocyclic inorganic linkers. **M.A. Omary**, R. Yasmeen, N.G. Rabah, S.M. Islam, C.M. Williams

1:30 575. Data-driven Analysis and Atomistic Simulations of Elecrical Conductivity in Two-dimensional Metal-organic Frameworks. **Y. Shi**, F.A. Shakib

1:45 576. Layer-by-layer assembly and structured color of Ti3C2Tz MXene/polyelectrolyte heterostructures. **N. Neal**, P. Stevenson, M. Radovic, M. Green, J. Lutkenhaus

2:00 577. Freeform additive manufacturing of carbon fiber reinforced composites using dielectric barrier discharge-assisted Joule heating. **S. Dasari**, M. Green

2:15 578. High-throughput screening, crystal structure prediction, and carrier mobility calculations of organic molecular semiconductors as hole transport layer materials in perovskite solar cells.. **M. Faruque**, S. Akter, D. Limbu, K.V. Kilway, Z. Peng, M. Momenitaheri

2:30 579. Synthesis and characterization of the novel Zintl Phase $Eu_{14}InAs_{11}$. **O. Pokhvata**

2:45 580. Impact of selected ionic liquids on the properties of metal halide perovskites. **M. Grubbs**, S. Dzyuba, J. coffer

3:00 Coffee Break.

3:30 581. From chemical expertise to AI precision: Progress in forensic fingerprint agent development and analysis. **J.L. Liu**, A. Enz, Z. Wang, S. Bashir

3:45 582. Upconverted Hot electrons in Mn-doped quantum dots can drive efficient solvated-electron mediated chemical transformation. **C. Orrison**, D. Son

4:00 583. Novel synthesis of modified ceria nanomaterials. **C.C. Watkins**

4:15 584. Sustainable Geopolymer Composite Reinforced with Natural Fibre: Preparation and Characterization. **Z. MOUJOUD**, A. El Bouari, O. Tanane

4:30 585. Crystal and electronic structure characterization of Ba_3As_2O and $Ba_{32}As_{23}O_2$, two new ternary barium oxyarsenide Zintl phases. **S. Watts**, L. Wingate, S. Baranets

Opportunities at the Interface of Academia and Industry

D. Anderson, *Organizer, Presiding*

Ranger 109

1:00 586. *Withdrawn*

1:30 587. Promote industry careers through academia and water sector collaborations. **H. Adams**, C. Fulton, M. Southard, J. Price, S. Reeder, C.A. Hansen, E. Appleton, J. Shao, D. Nix, K. Mahmud, B. Colvin

2:00 588. Bridging the Gap: AI-driven innovations in academic and industrial drug discovery. **D. Anderson**

2:30 Networking Break.

3:00 589. Translating research into innovations with impactful applications. **S. Anderson**

3:30 590. Closing the gap through entrepreneurial education. **S.M. Kerwin**

4:00 591. What now? Next steps for tech transfer and startup development. **L.E. Martinez**

4:30 Panel Discussion and Q&A.

Organic Chemistry (General)

N. Matsumoto, *Organizer, Presiding*

Texas 114

1:00 592. Stilbenes: Source plants, chemistry, biosynthesis, pharmacology, application, and problems related to their clinical application: A comprehensive review. **T.T. Teklehaimanot**

1:20 593. Synthesis, biological assessment and molecular docking studies of new pyrazolone compounds as potential anticancer agents against non-small cell lung cancer. **P. Anim Addo**, S. Murru, S. Dahal

1:40 594. Non-toxic polysaccharide-based anti-cancer drug delivery system utilizing Osajin and polymerized fenugreek seeds. **E. Soward**

2:00 595. Determination of Abraham summation solute hydrogen bonding acidity values for the catechol flavones. **W.L. Whaley**, M. Gregory, S. Tuck, M. Abraham, R. Srinivasan

2:20 596. Development and synthesis of methylene spacer functionalized prodrugs of TLR4-signaling inhibitor TAK-242 (Resatorvid) for controlled delivery. **C.A. Sells**, R. Gaykar, J.H. Kostyo, R.R. Kane

2:40 597. Photocatalyzed strain-release retro-Diels-Alder reaction. P. Das, **S. Kharbanda**, J.D. Weaver

3:00 Coffee Break.

3:30 598. New strategies for the synthesis of heterocyclic organotellurium compounds. K.M. Gaborit, A.K. Turner, S.R. Ponzo, F.R. Fronczek, **T. Junk**

3:50 599. *Withdrawn*

4:10 600. Synthesis, Structure, and Optical Properties of 8-Anilino BODIPYs. **K.H. Pannell**, A. Metta-Magana

4:30 601. *Withdrawn*

4:50 602. Synthesis and crystal structures of 18-crown-6 stabilized potassium salts of dioxalatodiphenylstannate and oxalatotriphenylstannate. **J. Sun**, **M. Rahman**, Y. Torres, T. Greaves, X. Song

Polymers and Sustainability Challenges 2

R. Foudazi, *Organizer, Presiding*

Ranger 106/107

1:30 603. Improving photovoltaic module lifetimes via creation of novel, low coefficient of thermal expansion backsheet polymers. **E.M. Redline**, E.M. Nagel, A.O. Scarlett, C.L. Staiger

1:55 604. Efficient photobase generators towards sustainable 3D printing. **Z.A. Page**

2:20 605. Spirocyclic inter-crosslinked polymer membranes: a materials platform to implement sustainable separations in gas and liquid phase. L.C. Condes, **M. Galizia**

2:45 606. Polymer films for sustainable solid-state capacitive energy storage and separation membranes. **A. Karim**

3:10 Intermission.

3:30 607. Polyelectrolyte solutions and brushes. **A. Marciel**

3:55 608. Ion-mediated reprocessable polymer thermoset. **S. Xie**

4:20 609. *Withdrawn*

4:45 610. High surface area crosslinked CNT-Microgel or CNT-CNT networks for sustainable agricultural and environmental applications. **Y. Gao**

5:10 Concluding Remarks.

Assessments for Learning and Engaging with Students

A. Sra, M. Stover, *Organizers, Presiding*

Ranger 110

1:35 Welcome and Brief Introduction.

1:40 611. In-state vs. out-of-state readiness for general chemistry. **D.S. Mason**, B. Mamiya

2:10 612. How word choice and phrasing can affect student performance in multiple choice assessments. **G.R. Dieckmann**, **S.M. Taylor**, B. Hefley, C.S. Tucker King, R. Davis, M. Islam

2:35 613. Using competency based assessment and a novel outcome framework to improve engagement in general chemistry. **J.A. Hebda**

3:00 Coffee Break.

3:30 614. Teamwork in the chemistry lab: instruction, practice and assessment. **E. Trufan**, E. Bouhoutsos-Brown

3:55 615. A novel way of teaching and assessing Organic II labs. **E.A. Nalley**

TUESDAY EVENING

Gooch-Stephens Award Lecture

J. Clinger, *Organizer, Presiding*
McLennan Hall

5:45 Introductory Comments.

6:00 616. Is a blind watchmaker the same as a blind neural net?. **A.D. Ellington**

6:55 Gooch-Stephens Award.

POSTER SESSIONS and EXPO and GRADUATE FAIR and RECEPTION

Brazos Ballroom

7:00 - 9:00 pm

Analytical Chemistry Poster Session

E. S. Gallagher, *Organizer*

617. From lab bench to career: Developing essential skills in chemistry labs. **E. Trufan**, E. Bouhoutsos-Brown

618. Analytical research & development at Merck: Leveraging diverse expertise to be partners in problem solving. **E.L. Schwalm**

619. Fiber-optic studies of the kinetics of myoglobin oxidation. **N.U. Dickson**, S. Mojeeb, D.E. Thompson

620. Optimizing tissue mimicking phantoms for gold nanorod photoacoustic imaging. **B.C. Fallon**, N. Mathuria, A. Martino, R. Bouchard, C.S. Filgueira

621. Nonlinear laser wave-mixing spectroscopy coupled with capillary electrophoresis and microchips for sensitive detection of SARS-CoV-2 biomarkers. **N. Shatirishvili**

622. Deep Ultraviolet Laser Ablation Electrospray of Proteins with Ion Mobility Mass Spectrometry. **K.B. Hines**, N. Feizi, T. Solouki, K.K. Murray

623. Comparing the ionization response factors of single-stranded DNA binding protein (SSB) oligomers bound to ssDNA using native mass spectrometry. **A.J. Blue**, M.G. Bannon, E.S. Gallagher, M.A. Trakselis

624. Molecular dynamics simulations of native-protein charging in electrosprayed droplets with experimentally relevant composition. **M.S. Cordes**, M.G. Bannon, E.S. Gallagher

625. Zn(II) affinity of a Zinc Finger Motif peptide model from competitive threshold collision-induced dissociation. **R.A. Adomako**, M.B. Owusu, K.N. Senyah, P. Asare, L.A. Angel

626. Comparing mice cardiac proteins extracted with different buffers using SP3 and SP4 clean-up methods. **S. Senarathne**, M.L. Law, E.S. Gallagher

627. Comparison of Byonic vs. GlycanFinder for identification and quantification of glycopeptides in biological samples. **V. Sandilya**, Y. Mechref

628. Chronic glyphosate exposure alters serum *N*-glycan profiles in rats. **M. Adeniyi**, C.D. Gutierrez-Reyes, J. Chávez-Reyes, B.A. Marichal-Cancino, J. Solomon, M. Fowowe, S. Onigbinde, J.A. Flores-Rodriguez, M. Al Amin Bhuiyan, Y. Mechref

629. Comparing solvents used for separation of carbohydrates in positive- and negative-ion mode mass spectrometry to improve ionization efficiency. **L.A. Garber**, A.N. Thurman, E.S. Gallagher

630. Characterizing carbohydrate isomers of varying size with in-ESI HDX-MS. **A.V. Quintero**, E.S. Gallagher

631. Utilizing Co^{2+} and electron-transfer higher-energy collisional dissociation to distinguish isomeric, sialylated human-milk oligosaccharides. **H.T. Wilson**, D.T. Gass, E.S. Gallagher

632. Identifying dysregulated lipids in human brain of Alzheimer's disease and their effects on biological pathways. **A. Sanni**, A.I. Bennett, M. Adeniyi, Y. Mechref

633. Lipid analysis of milk varieties using liquid chromatography-mass spectrometry. **S.W. Raja Hewage**, B. Williams, H. Fernando

634. Does Texas wildflower honey smell of Texas wildflowers? A GC-MS/O analysis. **M.J. Maguire**, T. Holland, K. Oyler

635. Metal removal and fractionation of asphaltene samples for multimodal characterization via derivatization for Kendrick Mass deficiency manipulation. **T. Thilakarathna**, B.A. Nyaaba, S. Makhani, T. Solouki, P.J. Farmer

636. Time-resolved extraction and quantitative detection of metals present in asphaltene samples: Using EPR, ICP MS, IM-MS, NMR, Synchronous Fluorescence, and UV-Absorption for asphaltene characterization. **B.A. Nyaaba**, T. Thilakarathna, S. Makhani, P.J. Farmer, T. Solouki

637. Direct lithium extraction from complex waste-streams based on electrochemical ion insertion in a 1D tunnel-structured positive electrode. **C.A. Larriuz**, J.L. Carrillo, A. Ezazi, H. Kohl, S. Banerjee

638. Lithium recovery from discarded lithium-ion batteries by electrodialysis. **K. Dumre**, C.P. Shelor

639. Unveiling synergistic dopants in copper, selenium manganese co-doped nickel sulfide metal organic framework electrocatalysts for superior urea electrooxidation and efficient hydrogen liberation:. **y. sana**

640. Preparation of copper oxide/(Cu-S)n metal-organic framework/reduced graphene oxide hierarchical structure for electrochemical quercetin sensing. S. Velmurugan, M. Tse, X. Lin, Y. Yu, **S. Cheng**, K. Lu

641. Analytical challenges and considerations for Iodine detection in Urine. **J. Girme**

642. Electrocatalytic properties of human liver subcellular fractions: Comparison of S9 fractions and human liver microsomes. **E. Alwarsh**, D. Medina, C.T. Walgama

643. Forbidden ion transport through cation exchange membranes. **C. Chaudhary**

644. Functionalization of high-density polyethylene capillaries for open tubular ion chromatograph. **E. Yousef**

645. Zirconia: Afluoride selective stationary phase for anion chromatography. **C. Warren**, P.K. Dasgupta, C.P. Shelor

646. Simple evaporative concentration method for the measurement of per- and polyfluoroalkyl substances in water matrices. **C.V. Odinaka**, C.P. Shelor

647. Probing the surface assembly of tetraphenyl porphyrin molecules linked with tin tetrachloride using atomic force microscopy. **Q. Do**, J.C. Garno

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Inorganic Chemistry Poster Session

M. AKRAM, *Organizer*

648. Exploration of s-block coordination chemistry via aggregation manipulation. **K. Martinez-Fair**, S. Yruegas

649. Accessing phenoxyimine calcium complexes via manipulation of the Schlenk equilibrium. **K. Birkhoff**, I. Lin, S. Yruegas

650. Isolation and reactivity of multidentate *s*-block carbene complexes. **D.N. Rodriguez**, S. Yruegas

651. Use of *para*-hydrogen to elucidate first-row reaction mechanisms. **B.M. Vaught**, A. Fout

652. Carboxylate-rich iron(III) complexes as phosphoesterase mimics in aqueous media. **E.T. Iqbal**, M.M. Mamori, H. Arman, G.T. Musie

653. Probing the influence of phenanthroline-based ligands on group 11 metal-ethylene complexes: discoveries and catalytic prospects. **D. Karade**, R. Dias

654. Photophysical studies of the three coordinate Cu(I) ß-diketiminate triphenylphosphine complexes. **A. Kumar**

655. Synthesis and primary characterization of Histidine-Salicylaldehyde metal complexes using microwave assisted technique. **D. Toole**, G. Chiarella, J. Ndongou

656. Ligand-to-ligand charge transfer (LLCT) transitions in square-planar metal-bipyridyl complexes of heteroatom-substituted maltol derivatives. **M. Usman**

657. Synthesis of antimony compounds with phosphorus and nitrogen based ligands. **L.D. Hale**, F.P. Gabbai

658. New fused-pincer ligand allowing the creation of novel bimetallic complexes. **J. Daum**

659. Using a Lewis basic bis-thiourea ligand to stabilize copper(I) complexes and explore oxygen activation. **S. Gupta**, A.R. Fout

660. Exploring the coordination chemistry of transition metal cobalt with pyrazole-based tripodal ligands. **J. Smith**, G. Lyubartseva

661. Complexation of a quinoline-based ambiphilic ligand platform to rhodium. **S. Bedajna**, F.P. Gabbai

662. Copper(II) phenanthroline complexes with polyphenols: Therapeutic agents for the treatment of hypertension and cardiovascular diseases. **V. Torres**, H. Arman, R.A. Adrian

663. *Withdrawn*

664. Novel cobalt(II) and copper(II) imidazole and phenanthroline complexes: Relationship between structure and antifungal efficacy. **O. Towers**, C.G. Pierce, H. Arman, R.A. Adrian

665. Synthesis and Characterization of Light-Triggered Metal Complexes for Cancer Treatment. **D. Lucas**, A. Talgatov, G. Shi, G. Kaur, A. Vali, C. Cameron, S.A. McFarland

666. *Withdrawn*

667. Investigation of the DSF/Cu reaction using LC HD MS. **j. lyons**

668. Approaches for optimization of the photodynamic therapy (PDT) efficiency with metallodrug photosensitizers in cancer treatment. **G. Shi**, A. Talgatov, A. Vali, D. Lucas, C. Cameron, S.A. McFarland

669. Synthesis and characterization of novel neodymium(III) bipyridine complexes: Structural analysis and theoretical correlation. **G.Y. Berrocal**, H. Arman, R.A. Adrian

670. Metal-Metal interactions in uranyl salophen-type complexes with the addition of early transition metals. **J. Ducilon**, J. Gorden, A.E. Gorden

671. Samarium(III) complexes with substituted 1,10-phenanthroline derivatives: Synthesis, characterization and crystal structures. **M. Cartwright**, H. Arman, R.A. Adrian

672. Lanthanide open networks incorporating derivatives of terephthalic acid. **D. Rios**, **E. Brandon**, **W. Best**, R.A. Zehnder

673. Lanthanide coordination polymers as surrogates to create isomorphous actinide counterparts. **T. Hodge**, **J. Turner**, R.A. Zehnder

674. Stabilizing ion pairs to access carbene-pyridine gallium complexes. **K.J. Francis**, S. Yruegas

675. Incorporating Lewis Acids into heterogeneous supports. **S. Ranasinghe**, C. Martin

676. Carborane-arene hybrid boron doped PAHs. **Y. Li**, M. Tamizmani, M. AKRAM, C. Martin

677. Improved solubility and the chlorination of the 1-*Closo*-Carborane Anion. **J. Raker**

678. Synthesis of azaborapyrenes from fused boroles. **A. Begum**, H. Zacharias, J. Han, T. Bartholome, T.B. Marder, C. Martin

679. Hydroboration of alkenes utilizing boronic acid catalysts. S. Mummadi, **R.L. Perry**

680. Exploring the reactivity of electrophilic boron compounds. **R. Thornton**, C. Martin

681. Polyborylated Lewis acids in Frustrated Lewis Pair (FLP) catalysis. **E. Sarkissian**, C. Krempner

682. Frustrated Lewis Pair Reactivity of Tris(*ortho*-carboranyl) Borane. **K. Vashisth**, S. Dutta, M. AKRAM, C. Martin

683. Stimuli-responsive donor-acceptor systems containing carbenium ions. **C. Lee**, F.P. Gabbai

684. Alloyed metal nanoclusters for triplet sensitizers. **K. Binkley**, S. Maiti, U. Ariyarathna, M. Kenari, A. Das

685. Enhancing PVDF triboelectric nanogenerators with $CuFeO_2$, $CuCoO_2$, $CuMnO_2$, and $CuGaO_2$ delafossites. A. James, **E. Varughese**, D. Phillips, F. Viesca, S. Mohan, M.J. Uddin

686. Impact of synthesis route on Ti_3C_2 MXene properties and applications. **S. Pas**, K. Arole, J.L. Lutkenhaus, M. Radovic, M. Green

687. Alloying-induced expansion in a metastable tunnel-structured cathode. **Y. Chiang**, P. Schofield, J. Ponis, S. Chakraborty, G. Agbeworvi, J.L. Carrillo, J. Ayala, B.J. Schultz, L. Gobbato, S. Banerjee

688. Redox-active Metalloligands as hosts for Cerium-based Photocatalysts. **Y. Shandilya**, S. Arnold, S. Phillips, K. Figueroa-Baez, O. Nachtigall

689. Advancing heteroanionicity in Zintl phases: Crystal structures, thermoelectric and magnetic properties of two quaternary semiconducting arsenide oxides, $Eu_8Zn_2As_6O$ and $Eu_{14}Zn_5As_{12}O$. **M. ISHTIYAK**

690. Leveraging lone pairs in search of fluoride-ion battery insertion anodes. **A. Pakhira**

691. Leveraging optically transparent porous salt thin films as a platform for solid-state organometallic chemistry and photochemistry. **S. Sarkar**

692. Disorder of Mn in Ce_2MnGe_6 and its effect on physical properties. **M. Raines**, B. Schundelmier, G. McCandless, K. Wei, J. Chan

693. Probing the limits of the Remeika tolerance factor. **R. Meduri**, A. Dominguez-Montero, J. Chan

694. Laser induced synthesis of cobalt oxide oxygen evolution catalysts. **A. Garza**

695. Synthesis, characterization, and photothermal effect of transition metal cobaltate nanoparticles deposited on nanographene oxide and nanographene.. **C.U. Ogbonna**, G. Neelgund

696. Synthesis and characterization of thiocyanate-capped copper ferrite nanoparticles. **D. Kumarage**, A. Picon, M. Escochea, S. Neugent, L. Marder, T.M. Trad

697. Controlling chemical and physical properties of tellurate inorganic pigments to achieve desirable colors and optical properties. **B. Amiri**

698. Developing eco-friendly coinage metal complexes using greener synthetic methods and natural materials as ligands for diverse applications. **H. Kouadio**, W. Ekhator, S. Banna, A. Tantish, D. Lene, Z. Taimuri, M. Rawashdeh-Omary

699. Investigation of Cu(II)-exchange reactions with a calcium tantalate. **M. Mongkhonratanachai**, **P.A. Maggard**, **S. Jana**

700. From insertion to interphases: Exploring the competition between fluoride-ion insertion and interphase formation in 1D tunnel-structured transition metal antimonites. **A. Giem**, W. Zaheer, S. Banerjee

701. Synthesis and characterization of dodecyl xanthate-capped magnetite nanoparticles and their bactericidal efficacy against *Xanthomonas* pathogens. **A. Picon**, L. Marder, D. Kumarage, S. Neugent, M. Escochea, T.M. Trad

702. Manganese doped Zinc Germanate (Mn:Zn2GeO4): Exploring a novel synthesis and its potential application in bioimaging. **D.A. Philips**, S.U. Shohag, B. Srivastava, S. Mohan, M.J. Uddin

703. Chemical vapor deposition synthesis of β-Gallium Oxide Nanostructures: Reaction Parameters' Effect on Morphology and Photoluminescence. **M. Jaekel**, L. Marder, T.M. Trad

704. Innovative approaches in low temperature material synthesis: Exploring crystal and electronic structures of novel metal cluster compounds composed of Ru, Os, and Bi. **G. Samarakoon Mudiyanselage**, S. Baranets

705. Novel Cis-Platin Alternatives with a Double-Headed Monster Action Against Cancer. **G.R. Calderon**, B. Adeyemi, M. Mehta, E. Skellam, M.A. Omary

706. Investigation of photoactive metallodrugs as antimicrobials. **G. Kaur**, A. Talgatov, G. Shi, A. Vali, C. Cameron, S.A. McFarland

707. Development of a web application for characterizing molecular vibrations for inorganic chemistry students. **O.M. Ayeni**, D. Omary, I. Migliaro, M.A. Omary, M. Atkinson

708. Redox cooperativity analysis with computational chemistry: Interplay between energy matching and geometric arrangement in redox non-innocent systems. **H. Watts**, J.B. Gary

709. Superhydrophobicity and Superhydrophobication Ability of Methylated Metal-Organic Frameworks (MeMOFs) and Hybrids Thereof as PFAS Alternatives for a Broad Spectrum of Apps. **O.M. Ayeni**, N.P. Davange, J. Fripp, M.A. Omary

710. Use of versatile luminescent complexes of Ruthenium(II) for moisture sensing. **B. Adeyemi**, J. Adebanjo, R. Perera, P. DiCarmine, M.A. Omary

711. Iridium- and rare earth-free amber/white/monochrome (O)LED solutions for video display/street or room lighting/traffic light apps. **D. Lene**, S. Li, Z. Lu, M.A. Omary

712. Beauty Beyond Jewelry: Glowing Gold Triangles as Genuine Metallointercalators. **N.G. Rabah**, A. Momeni, O. Valsson, M.A. Omary

P010. Highly emissive zero-dimensional hybrid antimony chlorides A_2SbCl_5 featuring long-chain cations. H. Majumder, **A.A. Miranda**, K. Thanabalasingam, K. McCall

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Physical Chemistry Poster Session

K. L. Shuford, *Organizer*

713. Analysis of microwave spectrum of Cyclopentanecarboxylic acid. **F. Jimenez**

714. Investigation of acetaldehyde photodissociation at 308 nm: Stereodynamics in competitive roaming. **D. Krongauz**, S.W. North

715. *Withdrawn*

716. Red Light Stress on *Chaetoceros* Diatoms. **K.C. Salaz**, J. Glenn-Millhouse, C.L. Waldie, A. Slover, S.C. Massey

717. Utilizing sum frequency generation spectroscopy to determine the ice nucleating mechanism of perfluorooctanoic acid. **L. Towers**, O. Curtin, J.D. Cyran

718. Red light and prolonged red light stress on *Phaeodactylum tricornutum*. **A. Slover**, **C.L. Waldie**, M.M. Nittala, M.Y. Buhari, K.C. Salaz, J. Glenn-Millhouse, S.C. Massey

719. Towards VENOM laser diagnostic technique to characterize multicomponent turbulent boundary layers. **T.B. Best**, S.W. North

720. Investigating the effects of low magnesium on *Phaeodactylum tricornutum* F710 fluorescence. **J. Glenn-Millhouse**, K.C. Salaz, A.K. Slover, C.L. Waldie, S.C. Massey

721. Characterization of hydrochar derived from *Chlorella pyrenoidosa* contaminated with copper and cadmium ion. **N. Smith**, K. Lasiter, C. Mitchell, B. Jang

722. Bacterial growth inhibition driven by surface phenomena of Microcrystalline Ga_2O_3 and GaO(OH). **D. Johnson**, P. Ahluwalia, P. Jodhka, A. Blom, J. Brannon, Y. Strzhemechny

723. Analysis of biosorption of heavy metal contaminated wastewater using kinetic and isotherm modeling for *Chlorella pyrenoidosa*. **K. Lasiter**, N. Smith, C. Mitchell, B. Jang

724. Experimental and computational studies of crystal violet removal from aqueous solution using sulfonated graphene oxide. **O. Oluwasina**, A. Adelodun, O. Oluwasina, H. Daurte, S. Olusegun

725. Formation of a silicon-carbon hybrid material from reacting silicon nanoparticles with acetylene. **G.J. Smith**, L. Canlom

726. Analysis of dispersed functionalized and non-functionalized single-walled carbon nanotubes. **D. Woodring**, **M. Schwickert**, B. Robinson, J.D. Beatty, N. Mirsaleh-Kohan

727. Surface tension measurements of charged microdroplets containing surfactants. **M. Johnston**, M. Jacobs

728. Molecular dynamics study of organochlorine ligand interaction with human serum albumin. **A. Mishra**, R. Yadav, D.S. Sanford

729. Impact of the SARS CoV2 viral fragment FI10 on amyloid β-42 aggregation. **M. Premathilaka**, A.D. Chesney, U. Hansmann

730. Identifying novel D-retro-inverso peptide inhibitors for mouse Serum Amyloid A 3 aggregation. **A.D. Chesney**, U. Hansmann

731. Analysis of SARS-COV-2 protein fragments on alpha-synuclein monomer conformations. **L. Coleman**, A.D. Chesney, U. Hansmann

732. Computational investigation of αCGRP monomers and interactions with SARS-CoV-2 spike protein fragment. **V.K. Anand**

733. Intrinsic energetics of proton transfer in concentrated binary $(HCl)_m(H_2O)_n$ clusters. **M. Tucker**, G.S. Tschumper

734. Revisiting the hydrogen halide dimers to probe the effects of sub-valence electron correlation. **Y. Xue**, G.S. Tschumper

735. Assigning the electronic absorption spectra of highly conjugated macromolecules. **H.A. Moran** , S. Kempel, Q. Michaudel, D.P. Tabor

736. Molecular insight on the hydration process of al-bearing species using density functional theory. **T. Fisher**, M.I. Malek, M.L. Pantoya, A. Aquino

737. An energy storage system that uses chemical bonds. **D. Medina**, S.A. Alexander

738. Vibrational polaritons revealed from infrared spectra by cavity quantum electrodynamical density functional theory within Gaussian atomic basis. **Z. Pei**, Y. Shao

739. Moving basis tensor implementation of Hierarchy of Pure states (HOPS). **B. Citty**

740. Spatially resolved fluorescence simulations of heterogeneous molecular semiconductors. **A. Hartzell**, T. Gera, D. Raccah

741. Ammonium perchlorate decomposition in the presence of TiO_2 anatase surface: a theoretical investigation.. **J. Zamora**, A. De Rezende, M.L. Pantoya, A. Aquino

742. Exploring the potential of Alloyed XMenes (aXMenes) for advanced energy applications: A computational study on stability and electronic properties. **P. Rijal**, U. De Alwis, K.L. Shuford

743. Finding molecules with large hyperpolarizabilities. D. Mashak, **S.A. Alexander**

744. Multireference calculations on bond dissociation and biradical polycyclic aromatic hydrocarbons as guidance for fractional occupation number weighted density analysis in DFT calculations. **J. Carvalho**, R. Nieman, M. Kertesz, A. Aquino, A. Hansen, H. Lischka

745. Quantum mechanical MP2 study of the electronic effect of nonplanarity on the carbon pyramidalization of fullerene C60. **Y. Liu**, Y. Gao, D. Liu

746. Modeling the chemiluminescence mechanism of ADLumin-5. **C. Wickizer**, C. Lander, Y. Shao, C. Ran

747. Charge transfer mechanism in excited states of boron/nitrogen doped polycyclic aromatic hydrocarbons. **L. Fonseca dos Santos**, F. Machado, A. Aquino, H. Lischka

748. Computational investigation of the thermal and photochemical mechanisms for the conversion of (TTP)Mo(η^2-O_2)$_2$ to (TTP)MoO_2. **C. Lander**, Y. Shao, K.M. Nicholas

P002. Targeted Inhibition of SARS-CoV-2 Main Protease (Mpro) Using Proteolysis Targeting Chimeras (PROTACs). **K. Chidambaranathan**, G. Sharma

WEDNESDAY MORNING

Inorganic Chemistry (General)

M. Akram, *Organizer, Presiding*

Texas 113

7:55 Introductory Remarks.

8:00 749. Guest inclusion into novel pillared hydrogen-bonded metal-organic frameworks. **G.A. Hogan**

8:20 750. Development of earth-abundant Cu(I)-photosensitizers using *N*-heterocyclic carbenes with variable anionic chelating ligands. **S. Chakraborty**, T.S. Teets

8:40 751. Synthesis and reactivity of base-supported organopnictogen Lewis acids. **N.H. Hunter**, F.P. Gabbai

9:00 752. Effect of metal, coligand, and number of thiophenes on the ground and excited state redox potentials of complexes of the type $[M(L)_2(IP\text{-}nT)]^{2+}$. **A. Vali**, A. Talgatov, H. Cole, G. Kaur, G. Shi, C. Cameron, S.A. McFarland

9:20 753. Development of non-classical photoprecursors for Rh_2 Nitrenes. **A. Paikar**

9:40 754. Dinuclear late-transition metal complexes of polyaromatic heterocycles. **U. Ekanayaka Arachchige**

10:00 Coffee Break.

10:20 755. Synthesis, characterization, and binding studies of new 1,3 benzotellurazoles containing a central pyridine units: Incorporation of chalcogen bond donors into a NNN pincer ligand.. **A. Amaya**, L. Delgado Cordoba, M. Abbasichaleshtori, H. Arman, A.F. Cozzolino, Z.J. Tonzetich

10:40 756. Applications of Photoactivated Metallodrugs for Cancer Therapy. **A. Talgatov**, D. Lucas, G. Shi, G. Kaur, J. Rahmon, D. Sunday, A. Vali, C. Cameron, S.A. McFarland

11:00 757. Bonding analysis of tetramethylguanidinyl arms supporting copper(I) catalytic sites. **J. Adebanjo**, Z. Lu, T.R. Cundari, P. Stavropoulos, M.A. Omary

11:20 758. Resonance-assisted hydrogen bonded fluorescent probe for relay recognition. **R. Mia**, B. Maillet, J. Weeks, M. Zepeta-Rodriguez

11:40 759. Photoreductive elimination of chlorine from a phosphine/oxaborine gold(III) complex. **P. Castro**, W. Liu, F.P. Gabbai

Emerging Topics in Environmental Chemistry

G. P. Cobb, C. M. Sayes, *Organizers, Presiding*

Lone Star 103

8:00 Opening Remarks.

8:05 760. Current status of micropollutants in aquatic environment. **V.K. Sharma**

8:30 761. Effect of the presence of emerging contaminants upon the compositional and functional dynamics of WWTPs sludge in Mexico. **L.G. Garcia Murillo**

8:55 762. New approaches to organofluorine sum parameter analysis. **C.P. Shelor**, C. Warren, C.V. Odinaka

9:20 763. Emerging tools for non-targeted analysis: Towards environmental decision making. **E.M. Ulrich**

9:45 Intermission.

10:00 764. Marine microplastic analysis: A case study of Matagorda Bay. **M.A. Azadah**

10:25 765. Mesoporous silica-based nanocarrier system as a strategy to deliver agrochemicals to plant crops. **X. Gao**, S. Ghoshal

10:50 766. Natural organic matter, from molecules to Earth. **C. Zhang**, M. Yan, G. Korshin

11:15 767. Insights into phosphate functionalization, kinetics, and mechanisim of phosphorylated sporopollenin as a sustainable catalyst for selective 5-hydroxymethylfurfural formation in water. **R. Sharma**, T. Selvaraj, V. Gowri, J. Varghese, J. Govindasamy

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Experimental and Computational Studies of Protein Structure and Dynamics

J. Clinger, *Organizer, Presiding*

Texas 117

8:00 768. Protein Bikram Yoga. **M. Fischer**

8:30 769. Interrogating proteins as molecular machines aided by machine learning. **P. Tao**

9:00 770. Active site electrostatics can gate enzyme dynamics during catalysis. **M.A. Wilson**

9:30 771. Molecular-dynamics simulations of protein crystals and diffraction data. **M. Wall**

10:00 772. Using deep learning and partial structure attention to solve the phase problem in crystallography. T. Pan, E. Dramko, M.D. Miller, A. Kyrillidis, **G.N. Phillips**

10:30 773. Lipid regulation of GPCR dynamics and ligand-receptor association. **B. Wylie**, E. van Aalst, J. Jang, S. Bannister

10:50 774. Quantum-mechanical molecular dynamics simulations of chemical reactions to investigate enzyme mechanisms. **R.A. Grove**, M.A. Wilson, A.M. Niklasson, C.F. Negre, M.E. Wall

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Materials for Energy and Environment

Cosponsored by ENFL

J. Larson, *Organizer, Presiding*

Texas 118

8:00 775. Novel hydrocarbon derived carbon nanomaterials for wearable and flexible printed micro-supercapacitors. **R. Banavath**, Y. Zhang, S. Deshpande, S. Dasari, M. Green

8:20 776. Covalent organic frameworks for rapid removal of perfluorooctanoic acid. **H. Vardhan**, R. Verduzco

8:40 777. Green-emitting Mn^{2+}:Cs_3CdBr_5 perovskite for WLEDs. **W. Yu**

9:00 778. Improved the photoelectrochemical stability and performance of $BiVO_4$ photoanode using In_2Se_3 as a protective layer in a harsh environment. **N.B. Belachew**

9:20 779. Metal quaterpyridine molecular complexes for photocatalytic CO_2 reduction on a crystalline carbon nitride scaffold. **S. McGuigan**, S.J. Tereniak, A. Smith, C.L. Donley, F. Zhao, S. Jeon, M. Pauly, L. Keller, L. Collins, S. Jana, S. Suhr, Y. Xu, N. Ghorai, H. Margavio, P.L. Holland, G. Parsons, T. Lian, E. Stach, P.A. Maggard

9:40 780. Unveiling the influence of cation mixing on photoelectrochemical water oxidation in $Mg_{1-x}Cu_xV_2O_6$ solid solutions. **A. Rawat**, R. Krishnan

10:00 Coffee Break.

10:30 781. Structuring V_2O_5 Positive Electrodes for Applications in Battery Cathodes and Direct Lithium Extraction. **J.L. Carrillo**

10:45 782. Fine-tuning microporosity of crystalline mixed-metal oxide frameworks for selective adsorptive separation of Kr from Xe. **S. Akter**, Y. Li, M. Kim, M. Faruque, Z. Peng, P.K. Thallapally, M. Momenitaheri

11:00 783. Effect of aluminum substitution ratio within nickel hydroxide cathodes for high performance alkaline nickel-zinc batteries. **J.A. Manley**, S.W. Kimmel, C.P. Rhodes

11:15 784. Lighting the path: Design principles for halide-ion solid electrolytes through spectroscopy and simulation. **J. Cheng**, S. Banerjee

11:30 785. *Withdrawn*

11:45 786. Low-temperature structural battery electrolytes produced by polymerization-induced phase separation. **S. Deshpande**, V. Vidyaprakash, S. Oka, S. Dasari, K. Liu, C. Wang, J. Lutkenhaus, M. Green

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Medicinal Chemistry

K. G. Pinney, *Organizer, Presiding*

Texas 115

8:00 787. Potent and selective small molecule PKCE inhibitors for non-opioid pain applications: Enantioselective synthesis, structure-activity relationship and *in vivo* efficacy studies. **S.F. McHardy**, H. De Kraker, C.N. Fleischer, A. Gregory-Flores, I. Magayewski Bonet, L. Barrera, H. Arman, R.N. Renteria, J. Levine, P. Parker, S. Kjaer, M. Marinelli, R.O. Messing

8:30 788. Evaluation of the cytotoxic properties of macrocyclic diterpenoids against triple negative breast cancer. J. Robles, **C.S. Fermaintt**

8:50 789. Design, synthesis, and biological evaluation of OXi8006 analogues bearing aryl ring bridge modifications as inhibitors of tubulin polymerization. **Y. Wong**, W.K. Rathnayake, C. Tamminga, Y. Deng, M.L. Trawick, R. Bai, E. Hamel, K.G. Pinney

9:10 790. Design, synthesis, and antimicrobial evaluation of some new thiopyrimidin-benzenesulfonamide compounds.. **S.H. Abdelwahed**

9:30 791. Site-selectively radiolabeled syndecan-1 antibody as a targeted radionuclide theranostics approach suitable for pancreatic cancer. **A. Yamaguchi**, R. Coll, Z. Yang, R. Ta, W. Yao, H.C. Manning

9:50 792. Strategies for selective delivery of vascular disrupting agents in the tumor microenvironment. **C. Pavlich**, W. Ren, Z. Shi, M.L. Trawick, K.G. Pinney

10:10 Coffee Break.

10:30 793. Synthesis of tripeptide drug-linker constructs cleavable by enzymes present in the tumor microenvironment. **K. Hamal**, Y. Wong, C. Pavlich, C. Borchardt, P. Tankoano, M.L. Trawick, K.G. Pinney

10:50 794. Unexpected directionality in thioamide hydrogen bonds stabilizes β-strands. **H. Zheng**, R.W. Newberry

11:10 795. Polygonum multiflorum: Recent updates on newly isolated compounds, potential hepatotoxic compounds and their mechanisms. **T.T. Teklehaimanot**, L. Wang, J. Gao, J. Mou, G. Pan, H. Yu, X. Gao, L. Han

Organic Chemistry (General)

N. Matsumoto, *Organizer, Presiding*

Texas 114

8:00 796. Cyclic and acyclic acetals as effective methylene sources for the synthesis of pillararenes. **B. Machireddy**, M. He

8:20 797. Asymmetric ruthenium-catalyzed carbonyl allylation and *tert*-prenylation via hydrogen transfer to π-unsaturated hydrocarbon feedstocks. **C. Saludares**

8:40 798. Dynamically generated carbenium species via photoisomerization of cyclic alkenes: Mild Friedel-Crafts alkylation. **O. Alkhamayseh**, T. Schoch, N. Herndon, E. Lantz, T. Fleske, J.D. Weaver

9:00 799. *β*-phenethylamine synthesis: *N*-pyridinium aziridines as latent dual electrophiles. **S. Samanta**, P. Biswas, B. O'Bannon, D. Powers

9:20 800. Development of a universal SuFEx reagent for deaminative C–C cross-couplings. **D. Chattapadhyay**, A. Aydogan, M. Diaz, Q. Michaudel

9:40 801. Triphenylborane Catalyzed [2+3]-Cycloaddition of Bestmann's Ylide, Ph_3PCCO, with Chiral Epoxides. **K. Nadella**, c. liu, C. Krempner

10:00 Coffee Break.

10:20 802. Synthesis of novel chemosensors: Bridged Calix[4]arenes and photoswitchable spyropyrans. **F.W. Foss**, R. Madigan, R.L. Miller

10:40 803. Reliable macrocycle molecular frameworks: Capitalizing on conserved conformations in triazine macrocycles. **C. Patterson-Gardner**, E. Simanek

11:00 804. Synthesis of prodrugs of AER-270 with controlled release kinetics. **A. Sarkar**, M. Nicosia, A. Valujskikh, R.R. Kane

11:20 805. Progress towards to total synthesis of (+)-pedrolide. **H. Shen**, J.L. Wood

Physical Chemistry (General)

K. L. Shuford, *Organizer*
U. De Alwis, *Presiding*

Texas 116

8:20 806. *Moved to 11:40 am in this session*

8:40 807. Molecules in oriented external electric field. **D. Lai**, D. Matthews

9:00 808. Generalizing electronic-vibrational couplings in the adaptive Hierarchy of Pure States (adHOPS). **J.K. Lynd**, D.I. Raccah

9:20 809. DFT study on the catalytic mechanism of N_2 reduction by a borylene complex. **S. Yu**, M.B. Hall

9:40 810. Computationally assessing electron-withdrawing chalcogen bond donors in N_2 activation chemistry. **K.A. French**, V. Choutipalli, K.L. Shuford

10:00 Coffee Break.

10:20 811. Ligand characterization and DNA intercalation of Ru(II) polypyridyl complexes: A local vibrational mode study. **H. La Force**, M. Freindorf, E. Kraka

10:40 812. Astrochemical modeling of acetonitrile chemistry in the interstellar medium: A computational study. **K. Fleming**, E. Kraka

11:00 813. Automated atomic grids in least-squares tensor hypercontraction. **C. Yin**, J.H. Thorpe, D.A. Matthews

11:20 814. Uranium-ligand bonding in uranyl-peroxide dimers and uranyl-hydroxo dimers: A local vibrational mode pilot study. **D. Gamage**

11:40 806. Organization of mixed self-assembled monolayers: Case studies in adsorption and aggregation of biomolecules, inorganic catalysts, and petroleum mimics. **R.S. Thompson**, O. Guzman, I. Guzman, J. Godino, E. El-Shaer, L. Garcia, A. Havens, R. Escobedo, L. Payne, A. Nesheiwat, G. Caswell, L. Kandil

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Analytical Chemistry (General)

E. S. Gallagher, *Organizer, Presiding*

Lone Star 104

8:30 815. Characterization of volatiles emitted from 3D printed polymers: Implications for ghost gun manufacturing. **H. Browning**, J. Carrell, P. Tiedemann

8:50 816. Chemical analysis of electronic nicotine delivery systems. **j. mata**

9:05 817. Surrogate optimization for supercritical fluid extraction-supercritical fluid chromatography hyphenated mass spectrometry. **N. Bhakta**

9:25 818. Acoustofluidics for separation and purification of heavy metal adsorbed MPs in the aquatic environment. **N.A. DeSilva**, M.E. Piyasena, N. Perera

9:45 819. Analysis of eggshell health of East Texas landfowl and waterfowl. **C. Davis**, A.S. Frantzen, F. Majs

10:00 Coffee Break.

10:30 820. Effect of the substituent groups of Tyr_5 and His_6 on the gas phase zinc affinities of acetyl-His_1-Cys_2-Gly_3-Pro_4-X_5-X_6-Cys_7 heptapeptides. **M.B. Owusu**, R.A. Adomako, P. Asare, K.N. Senyah, R. Oberdick, L.A. Angel

10:50 821. Retention-time alignment and imputation algorithms affect statistical comparisons when multiple samples are searched together in proteomics database searching software.. **J.M. Conforti**, C.C. Breus, C.S. Worth, J. Taube, E.S. Gallagher

11:10 822. Application of binomial distribution statistics for quantitative proteomic analysis. **S. Momin**, T. Solouki

11:25 823. Urinary fatty acid biomarkers for prostate cancer detection and prognosis. **E. Noriega Landa**, G. Quaye, W. Lee, X. Su

11:45 824. Variations in intracellular organometallic reaction frequency captured by single-molecule fluorescence microscopy. **G. Yan**, D. Nguyen, T. Chen, L. Do

Advances in Polymer Chemistry

J. A. Irvin, *Organizer*
M. Sheokand, *Presiding*

Ranger 106/107

8:55 Welcome.

9:00 825. On-demand drug delivery via photothermal stimulation of dynamic covalent poly(ethylene glycol)/PEDOT hydrogels. K. Thapa, M. Otakpor, A. Strait, E. Rodriguez, S. Bhuiyan, Y. Kinfe, T. FitzSimons, N. Conrad, A. Crowell, A. Rosales, **T. Betancourt**

9:20 826. Synthesis and application of electrochemically-active sequence-defined oligourethanes towards long-term data storage. **B. Pandey**, B. Muralidharan, E.V. Anslyn

9:40 827. Accessing sustainable polysulfamates through sulfur(VI) fluoride exchange (SuFEx) polymerization. **S. Das**, K. Doktor, Q. Michaudel

10:00 828. Leveraging steric effects in monomer design to access precise pyridine-containing polymers via ROMP. **A. Tran**, Q. Michaudel

10:20 Intermission.

10:40 829. Mechanistically-informed stereoselective ring-opening metathesis polymerization for precise synthesis of poly(*p*-phenylene vinylene)s. **J. Nicholson**, S. Kempel, Q. Michaudel

11:00 830. Continuous flow synthesis of polar polyethylene block copolymers. **S. Sarkar**, H. Dau, E. Harth

11:20 831. Closing the loop for Polyacylhydrazone(PAcHy) soft materials. **M.B. Minus**, C. Ufodike, A. Rahman, E. McHenry, M. Giles, G. Nzebuka

WEDNESDAY AFTERNOON

Advances in Polymer Chemistry

J. A. Irvin, *Organizer*
T. Betancourt, *Presiding*

Ranger 106/107

1:00 832. Vapor phase deposition of electroactive polymers onto electrospun commodity polymer nanofibers. **S. Brahma**, N.R. Lontkowski, J. ur Rehman, T. Betancourt, J.A. Irvin

1:20 833. Tensile behavior of electroactive polymer coated polyacrylonitrile nanofibers. **A. Gustafson**, J.A. Irvin, K. Bay, S. Brahma, A. Libonati

1:40 834. Bio-sourced adhesive with fire protection. **D.L. Smith**, D. Rodriguez-Melendez, M.O. Convento, M. Montemayor, J.C. Grunlan

2:00 835. Fully biobased and biodegradable oxygen barrier coating for poly(lactic acid). **S. Fisher**, E. Iverson, E. Chang, J.C. Grunlan

2:20 836. Effects of alkyl polgyglucoside tail length on surfactant foaming properties. **G.R. Overholt**

2:40 837. Solvent-Induced Mobility of Polymer Chains and Metallocene Migration into LDPE: A HRMAS NMR Study. **M.R. Kimball**, J.C. Hoefler, J. Bluemel

Environmental Chemistry and Toxicology

G. P. Cobb, C. M. Sayes, *Organizers, Presiding*

Lone Star 103

1:00 Open Discussion.

1:05 838. Inductively coupled plasma-mass spectrometry (ICP-MS) preparation techniques for solid-state sample analysis. **M. Stevens**, C.M. Sayes

1:30 839. Moved to Monday poster session #P005

1:55 840. Study of microplastics in wastewater treatment plants in deep east Texas. **J. Swallow**, K.K. Onchoke, R. Friedfeld

2:20 841. Determining the degradation rate of polystyrene microplastics after reacting with Amano lipase, manganese peroxidase, and Fenton oxidation.. **J. Lugo**, T. AYORINDE, A. Charlton-Sevcik, C. Sayes

2:45 842. Quantification of microplastics in soil and mulch. **C. Hyppolite**, T. Phan, A. Bastidas, K. Miller, I. Simon, V. Tran

3:10 843. *Withdrawn*

3:35 844. Biodiesel vs conventional diesel: An analysis of particulate matter formation. **C.C. Watkins**

4:00 Introductory Remarks.

Inorganic Chemistry (General)

M. Akram, *Organizer, Presiding*

Texas 113

1:00 845. Extraction and synthesis of the active components of inorganic sunscreen. **C.C. Watkins**

1:20 846. Designing Metal Halides for Fast Neutron Imaging: Chain-Head Engineering in Hybrid A_2MnCl_4 Emitters. D. Banerjee, E.J. Brand, **K. McCall**

1:40 847. Efforts to improve crystallization protocols of an unknown plutonium compound to allow for its full structural characterization. **R.A. Zehnder**

2:00 848. Design Principles for Cooperativity in Redox Processes. A. Henderson, H. Watts, A. Telford, M. Garcia Dalmases, C. Young, E. Ah Leong, L. Kimble, S. Shipman, B.M. Barngrover, **J.B. Gary**

2:20 849. Structure, activity and stability of ruthenium-chromium oxide aerogel oxygen evolution electrocatalysts. **J. Adame Solorio**, S.W. Kimmel, C.P. Rhodes

2:40 850. Antimony(V)/crown ether conjugates as cation-anion symporters. **A. Kim**

3:00 Coffee Break.

3:20 851. Creating solid solutions of ferrocene, cobaltocene, and nickelocene: A paramagnetic solid-state NMR study. **G. Harmon**, V. Bakhmutov, J. Bluemel

3:40 852. Low temperature synthesis, crystal and electronic structures of Osmium & Ruthenium Chalcobromides : $Os_2S_4Se_2Br_{10}$, $Os_2Se_6Br_{12}$ & $Ru_2Se_6Br_{10}$. **T. Kandabadage**, S. Baranets

4:00 853. Joule heating as a high-temperature out-of-oven manufacturing technique for nanocarbon/inorganic composites. **S.T. Upama**, A. Mikhalchan, L. Arévalo, A. Pendashteh, J. Vilatela, M. Green

4:20 854. Aerobic oxidation of hydrocarbons using site isolated vanadyl in Metal Organic Frameworks. **T. Ericson**, M. Ghartemani, J. Emanuele, S. Khatib, A.F. Cozzolino

4:40 855. Structure and performance of high-energy ball milled iridium-titanium oxide oxygen evolution electrocatalysts. **K.R. Bailey**, J. Adame Solorio, C.P. Rhodes

Metalloenzyme Design

I. V. Korendovych, *Organizer, Presiding*
L. R. Marshall, *Presiding*

Texas 117

1:00 856. Peroxidase behaviors of heme-amyloid species. **L.R. Marshall**, O. Zozulia, I. Kim, E.M. Kohn, I.V. Korendovych

1:30 857. Uno Ferro, a de novo designed protein, binds transition metals with high affinity and stabilizes semiquinone radical anion. **O. Makhlynets**

2:00 858. *De novo* design of protease-activated antimicrobial proteins. **S. Bhattacharya**, W.F. Degrado

2:30 859. Catalytic nanoassemblies formed by short peptides promote highly enantioselective transfer hydrogenation. **I.V. Korendovych**

Organic Chemistry (General)

N. Matsumoto, *Organizer, Presiding*

Texas 114

1:00 860. Concise total synthesis of the psammaplysin alkaloids. **A. Morrow**

1:20 861. *Withdrawn*

1:40 862. Vitamin B_{12}-catalyzed cyclopropanation reactions. **J. Teye-Kau** , S. Pitre

2:00 863. Molecular motors driven by electrons and protons. **Y. Feng**

2:20 864. Halogen-bonding photocatalyzed radical perfluoroalkylation reactions. **T. Tasnim**, S. Pitre

2:40 865. Bioorthogonal engineering of trehalose-modified glycolipids in mycobacterium: Unraveling molecular interactions via click chemistry. **D. Czapski**

3:00 Coffee Break.

3:20 866. Electronically mismatched Diels-Alder reaction via Lewis Acids catalyst. **M. Qureshi**, S.R. Hussaini

3:40 867. Phthalimide addition to styrene oxide or glycidyl phenyl ether using ammonium salts as catalysts. **C.J. Neef**, E. Hammeke, C. Wheeler, H. Humes

4:00 868. *Withdrawn*

4:20 869. Co-catalytic coupling of alkyl bromides and chlorides: The curious role of Lutidine. **P. Sharma**, R. Hanumanthu, A. Ethridge, J.D. Weaver

4:40 870. Cu-catalyzed strain-release-driven radical difunctinalization reactions of unsaturated compounds. **A. Popov**, V. Viviani, P. Skumial, T.L. Jefferson, S.G. Salman, H.H. Baxter, K. Hull

5:00 871. Mechanochemical synthesis of enamino carbonyl compounds.. **M. Ndlovu**, S.R. Hussaini