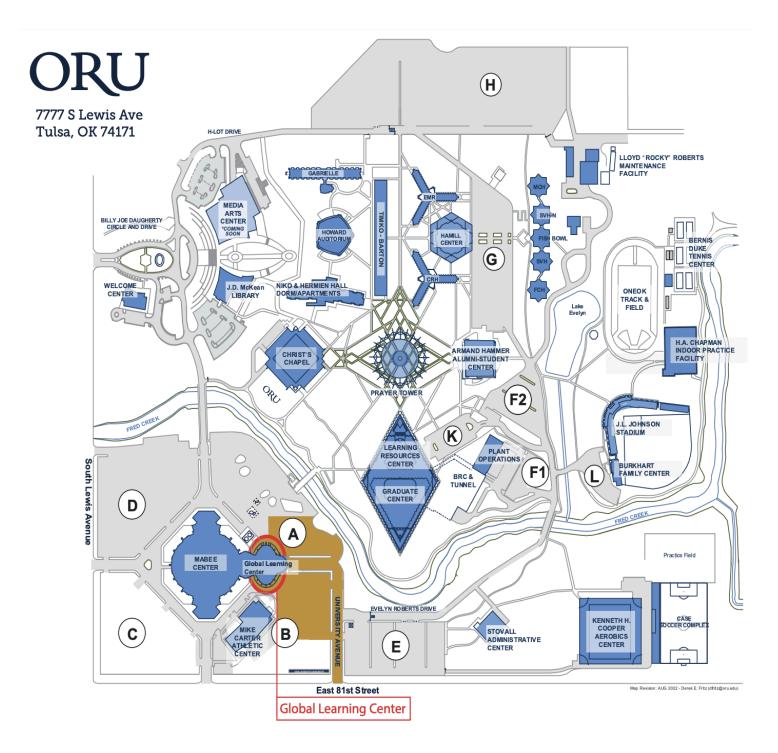


66th Annual Oklahoma Pentasectional Meeting of the American Chemical Society

March 1st, 2025 Oral Roberts University Tulsa, OK



Meeting will be held in the Global Learning Center Oral Roberts University 7777 S Lewis Ave, Tulsa, OK 74136

Schedule of Events

On-site Registration and Check-In	9:00-9:30 am
Poster set-up for morning session	9:30-10:00
Welcoming remarks (GLC 100)	
Dr. Kenneth Weed, Dean of the College of Science and Engineering	9:45-10:00
Technical sessions (morning)	
Session 1 - GLC 203 (Analytical/Physical)	10:00-12:00
Session 2 - GLC 102 (Biochemistry)	10:00-11:40
Session 3 - GLC 101 (Organic)	10:00-12:00
Session 4 - GLC 103 (Materials/Polymer)	10:00-11:20
Poster presentations (morning)	10:00-12:00
3 rd Floor, GLC	
Lunch (GLC 100)	12:00-1:30
Presentation of Oklahoma Chemist of the Year	
Poster set-up for afternoon session	1:30-2:00
Technical sessions (afternoon)	
Session 5 - GLC 101 (Inorganic/Analytical/Physical)	2:00-3:40
Session 6 - GLC 103 (Physical/Materials)	2:00-3:20
Session 7 - GLC 102 (Organic)	2:00-3:40
Session 8 - GLC 203 (Biochemistry)	2:00-3:20
Poster presentations (afternoon)	2:00-4:00
3 rd Floor, GLC	
ACS Officer Pentasectional Organizational Meeting GLC103	4:00

2025 Oklahoma Chemist of the Year

Frank Blum, PhD

Frank became Department Chair of Chemistry at Oklahoma State University in the Fall of 2009. He currently serves the Harrison Bartlett Chair and Regents Professor of Chemistry. Previously he spent five years at Drexel University and 24 years at the University of Missouri-Rolla (UMR)/Missouri University of Science and Technology (MS&T).

As Chair, Dr. Blum led the OSU chemistry department to grow and diversify. The diversification has enhanced Oklahoma chemistry through the development of role models for an increasing diverse student body. With 13 faculty hires, the Department has undergone many positive changes. These and other outreach efforts enhanced the standing of the department within the college, campus, and external shareholders, especially alumni. During this time, several new gifts from alumni and friends enhanced support for chemistry students.

As an Educator at OSU, Frank has taught general chemistry courses with hundreds of students, intermediate classes in physical chemistry, and smaller classes for graduate students in polymer chemistry/science, spectroscopy, physical chemistry and colloid chemistry. He also developed a new course, Introduction to Chemistry Research for incoming graduate students, to help new students understand their environments, departmental facilities, interactions with advisors, and other important functions. He has also developed a set of elective courses for chemical professionals including: The Periodic Table (the idea came from Professor Vasquez); What's That Stuff; The Chemistry of Life; and The Chemistry of Materials. These have become very popular with students and faculty and, in addition to providing more information on practical chemistry, and gives students the opportunity to work on writing and presentations. In his classes, he focuses on how chemical lessons relate to students' majors, our society and world.

In research, Dr. Blum has made major contributions in the understanding of how polymers interact with solid substrates and his group have characterized the behavior such as heat capacity of very small amounts of polymer at the interface, (as thin as 1 nm or so). The Blum lab has shown how to make synthetic polymer composites at room temperature, which normally require high temperatures for preparation, thus making composites which can contain active enzymes. They helped develop the technology for and understanding of superhydrophobic coatings. In the last few years, they have also developed the technology for making useful composites from post-consumer carpets and bottle waste parts, which have the potential for reducing the impact of these materials in the waste stream. In performing this research, at Drexel, MS&T and OSU, his students have successfully completed 39 Ph.D. theses and 21 master's degrees. He has also advised five co-advisees in engineering and physics, ten undergraduate researchers, six high school students, and 14 post-doctoral and visiting scholars.

Service at all levels has been a hallmark of Frank's professional life. He has been heavily involved in ACS National activities in nominations, awards, publications and the ACS Council. Important aspects of his service efforts have been in Oklahoma. He has participated in the Oklahoma Pentasectional Meetings. He and his students have presented 32 papers at the Pentasectional Meetings, including in 2013-Tulsa, where he gave the Plenary Lecture on "Tough Stuff: - The Polymer Age". He has cherished these meetings and discussed their impact with members of the ACS Board of Directors.

Frank has lectured in every Oklahoma Local Section at meetings, colleges/universities and companies, plus several in surrounding areas in Kansas and Texas. He has also been a reviewer for the ACS in the region for the Chemistry programs at Northeastern University, the Polymer Program at Pittsburg State University and also the Chemistry Department at the University of Arkansas.

Frank was one of the main organizers for the Southwest Regional ACS Meeting in 2023 (SWRM23) and primarily served as the main Program Chair. Working with ACS and others, the OK Local Section became incorporated and the SWRM23 LLC was formed with Cheryl Frech, Lloyd Bumm, and Frank Blum as the Directors. Within the program, about 50 symposium organizers closely worked with him. The venue was packed with programming including 54 technical sessions. Each session was designed with two co-organizers, typically one from inside Oklahoma and one from outside the state to act as a liaison (ambassador) in their local area. This worked well, and the meeting attracted over 1000 attendees. Two other significant events in the meeting were a pre-meeting social with tour at the new First American's Museum in OKC and a symposium on Diversity which were considered highlights of the meeting.

At SWRM2023, the symposium on Best Practices for Successful Small Chemical Businesses was originally planned to be organized by Allen Apblett. His untimely death required action and Frank assisted as a behind-the-scenes organizer. The symposium was a great success and included presentations highlighting Oklahoma Small Businesses including: Carol Hintzel from Mega Molecules (OKC), Sharina Perry, Utopia Plastix (OKC), Nick Materer from Explosafe (Stillwater), and Stewart Kennedy from Dry Surface Technologies (Guthrie) as well as others with Oklahoma connections embedded in the rest of the technical program from companies like Chevron Phillips, Hempel, Phillips66, Albemarle, and Covestro.

Dr. Blum's research group has been extremely effective in working with Oklahoma Companies providing technical support for them. These include Dry Surface Technology (Guthrie, OK), MITO Material Solutions (Stillwater, OK and Indianapolis, IN), and Zero Plastics (Tulsa, OK). These interactions support the broader land-grant mission of the university. Additionally, Dr. Blum was a key participant in the City of Stillwater's decision to build a new recycling center in Stillwater. He gave a presentation to the Stillwater City Council on the Citizen's Task Force on Recycling. This effort helps keep environmental issues moving forward.

In conclusion, Dr. Blum has had a significant impact on many aspects of promoting chemistry in the State of Oklahoma, the region, and the world-wide chemical community.

Oklahoma Chemist History

The Oklahoma Chemist Award was initiated in the early 1970s and was primarily started by Dr. George R. Waller who was a faculty member in the Biochemistry Department at Oklahoma State University. Oklahoma is divided into five sections of the American Chemical Society, and each Section agreed to support this award on an annual basis. The concept for the award was to honor truly outstanding contributions made to science and to the state by a chemist in recent years within the State of Oklahoma. Although originally designed to honor research chemists, an amendment was introduced in the 1980s to allow candidates to be nominated who had made extraordinary contributions to the area of chemical education whether it be to youth or to the public in general. Three such awards have been made to chemical educators over the years since the inception of the award in 1971. One award was to be given each year if a suitable candidate was identified from the research community or from education. The original award consisted of \$500 and a handsome plague. One member from each of the five Sections was appointed to compose a reviewing committee to accept nominations which were to be received around February 1 of each new year. The date was to permit sufficient time for the winner to be selected and to receive the cash award and plaque at the next annual Pentasectional Meeting in the spring. The Pentasectional Meeting brings together chemists from academia and from industry within the state one time each year to present research results. It is the largest meeting of chemists in Oklahoma. The Oklahoma Chemist Award is the most prestigious award given to a chemist within Oklahoma. The award now consists of \$1000 as well as the plaque described above. A brief description of the accomplishments by the recipient are engraved on the plaque and are submitted, along with a photo of the winner, to Chemical and Engineering News for official publication in a forthcoming issue. Chemical and Engineering News is a major publication of the American Chemical Society and has world-wide distribution. The Oklahoma Chemist Award is sponsored by the five Oklahoma Sections of the American Chemical Society with the additional support of the chemical industries in the State of Oklahoma.

OKLAHOMA CHEMIST AWARDEES

1971 Wayne White, Ozark-Mahoning Company, for developing commercial processes for stannous fluoride and sodium monofluorophosphate, the two fluorides most widely used as dentifrice additives.

1972 No award

1973 Otis C. Dermer, Oklahoma State University, for his outstanding service to the people of Oklahoma in building a first-rate Chemistry Department at Oklahoma State University and for his nationally recognized contribution to the chemical nomenclature and chemical education.

1974 Robert L. Banks, Phillips Petroleum Company, in recognition of his outstanding contributions to the field of chemistry in the olefin disproportionation reaction and in catalysis.

1975 Charles M. Starks, Conoco, Inc., in recognition of and publications on phase transfer catalysis.

1976 Kang Yang, Conoco, Inc., in recognition of his scientifically sound and innovative theoretical concepts in radiation chemistry, photochemistry, rate theory, electrochemistry and catalysis, and application of chemical kinetics to these concepts.

1977 Kenneth Darrell Berlin, Oklahoma State University, in recognition of his many, and significant contributions to heterocyclic phosphorus chemistry.

1978 Gerard Kraus, Phillips Petroleum Company, for his outstanding contributions to the physical chemistry of industrial polymers.

1979 Lionel M. Raff, Oklahoma State University, for pioneering work in the use of theoretical chemical physics as a practical tool for electrical structures, reaction rates, and energy transfer processes.

1980 Wayne F. Hower, Halliburton Services, for invaluable contributions to the science and practice of well completions and well stimulation methods in the petroleum and related industries.

1981 Alfred Clark, retired from University of Oklahoma after retirement from Phillips Petroleum Company, in recognition of outstanding contributions to theory and applications of adsorption and catalysis.

1982 Marvin M. Johnson, Phillips Petroleum Company, in recognition of his many innovative contributions in the areas of metal passivation on cracking catalysts and reclamation of used motor oil.

1983 Simon Wender, University of Oklahoma, for his contributions to the understanding of the chemistry and biochemistry of plant phenolics.

1984 E. J. Eisenbraun, Oklahoma State University, in recognition of his many contributions in the field of natural products and high purity organic chemicals.

1985 Dick van der Helm, University of Oklahoma, in recognition of his contributions in the field of structural analyses by x-ray crystallography.

1986 Sherril D. Christian, University of Oklahoma, in recognition of his contributions to the field of colloid chemistry.

1987 Francis J. Schmitz, University of Oklahoma, for his achievements in the isolation, characterization, and pharmacological applications of marine natural products.

1988 Marvin K. Kemp, Amoco Production Company, for his contributions in developing and expanding the science enrichment program for fourth and fifth grade students, education, and practical geochemistry research applications.

1989 Glenn Dryhurst, University of Oklahoma, in recognition of outstanding achievements in the field of chemical research and education in the state of Oklahoma.

1990 Horace A. Mottola, Oklahoma State University, in recognition of his contributions in the areas of continuous flow kinetics and immobilized enzymes.

No award

Elizabeth Anne Nalley, Cameron University, in recognition of her contributions to the teaching of chemistry to grade school, high school, and college students.

Bing M. Fung, University of Oklahoma, in recognition of his contributions in the fields of liquid crystals and nuclear magnetic resonance spectroscopy.

No award

Gilbert J. Mains, Oklahoma State University, in recognition of his contributions in the fields of photochemistry and computational chemistry and as an educator.

Max P. McDaniel, Phillips Petroleum Company, in recognition of his contributions to olefin polymerization catalysis and the polyethylene industry.

Donald L. Thompson, Oklahoma State University, for pioneering work in molecular dynamics and contributions to chemistry in Oklahoma.

1998 Roger E. Frech, University of Oklahoma, for his contributions in the research of solid-state ionic materials, teaching and mentoring students, and establishing cooperative research centers with other Oklahoma scientists.

Warren T. Ford, Oklahoma State University, for his outstanding contributions in polymer chemistry.

2000 Robert E. Howard, University of Tulsa, for outstanding contributions to chemical education at the elementary, secondary, and college levels.

George R. Waller, Oklahoma State University, for outstanding contributions to biochemistry, mass spectrometry, and natural product chemistry.

2002 P. K. Das, Phillips Petroleum Company, for outstanding contributions to computational methods for catalyst design with emphasis on the development and characterization of metallocene- based polyolefin catalysts.

2003 James Weaver, Halliburton Research Services, for contributions in chemistry for improving petroleum production efficiency and worker safety with minimum environmental impact.

Daniel E. Resasco, University of Oklahoma, for outstanding contributions in nanotechnology and in petroleum refining.

2005 Neil Purdie, Oklahoma State University, for outstanding contributions in chemical education at the university level and for the development of a computer program for assisted analysis of lipid profiles.

2006 Donald D. Knudsen, ChevronPhillips Company, for outstanding contributions to the field of polyolefin catalysis and outstanding leadership and technical expertise in the development and commercialization of selective 1-hexene technology.

2007 Ziad El Rassi, Oklahoma State University, for outstanding contributions to chemistry in the state of Oklahoma in the field of chromatography, especially in the area of liquid phase separation techniques.

2008 Joe Allison, Conoco Company, for outstanding contributions to chemistry over broad areas spanning the oil, gas, and chemical industries and his significant service to the ACS on both the local and national levels.

2009 Richard A. Bunce, Oklahoma State University, for outstanding contributions to synthetic organic chemistry and the development of tandem reactions for the synthesis of carbocyclic and heterocylic systems.

2010 Jiten Chatterji, Halliburton Energy Services, for outstanding contributions in the areas of cementing and fracturing in the industry of oil recovery.

2011 Dale Teeters, University of Tulsa, for outstanding contributions in fabrication and characterization of electrolyte systems in nanoporous membranes.

2012 Donna Nelson, University of Oklahoma, for outstanding contributions in unifying additions to alkenes via physical organic chemistry, determining SWCNT functional group molecular level interactions, quantifying research university STEM faculty demographics, and chemical advising to congress, television, and professional organizations.

2013 Tushar Choudhary, Phillips 66 Research Center, for outstanding work in clean fuels optimization, diesel hydrotreating catalysis, catalyst development for gasoline desulfurization, clean hydrogen production for fuel cell applications, and oxidation catalysis.

2014 Allen W. Apblett, Oklahoma State University, for outstanding contributions in chemical research, education, leadership, and entrepreneurship in the state of Oklahoma.

2015 A. K. Fazlur Rahman, Oklahoma School of Science and Mathematics, for outstanding contributions in chemical education and leadership at the secondary level and the college level.

2016 Frankie Wood-Black, Director of Process Technology at Northern Oklahoma College and Principal of Sophic Pursuits, Inc., for outstanding contributions in the oil and gas industry and in chemical education from the elementary to college level in the State of Oklahoma.

2017 Dwight L. Myers, East Central State University, for outstanding contributions in chemical education at the college level.

2018 Robert E. Anderson, University of Oklahoma Health Sciences Center, for outstanding contributions to the understanding of the role of lipids in visual function, the discovery of the importance of docosahaenoic acid in retina function, and for mentoring students.

2019 Kenneth M. Nicholas, University of Oklahoma, for outstanding contributions to the discovery, fundamental understanding and applications of chemical reactions promoted by transition metal compounds.

2020 Kenneth Roberts, University of Tulsa, for Outstanding Contributions to Chemical Education and Research in Water Chemistry

2021 No Award

2022 Tim Hubin, Southwestern Oklahoma State University, for stellar mentoring of undergraduate research and outstanding contributions to chemistry education.

2023 George Richter-Addo, University of Oklahoma, for his stellar research of nitric oxide interactions with biological metals and for contributions to chemical education in the state of Oklahoma.

2024 No Award

2025 Frank Blum, Oklahoma State University, for his stellar research on polymers and surface-active materials and for advancing the chemistry community in the State of Oklahoma.

Morning Presentation Schedule

Session 1 - Analytical/Physical - Room 203, Global Learning Center	<u>er</u>
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Session Chair: Dr. Lloyd Bumm

10:00-10:20 (A1) Au Magic Fingers in Air: Solvent-Driven Nanostructure Formation on Au(111)

Nazila Hamid, Dillon Dodge, Rowan Dirks, Lauren F. Hornbrook,

Erin V. Iski

The University of Tulsa

10:20-10:40 (A2) Catalytically Relevant Charge Transfer Reactions at Metal-Organic

Framework-Liquid Interfaces

Hyunho Noh, N. Gökçe Altınçekiç, Hafsa Abdul Ghuffar, Chance W. Lander,

Zachary J. Ingram, Miguel A Liuzzi-Vaamonde, Anne Martin Salazar

University of Oklahoma

10:40-11:00 (A3) Mechanical Exfoliation and Optoelectronic Characterizations of

1,4,8,11,15,18,22,25-octabutoxyphthalocyanine Thin Films

Steven M. Raybould, Lucas Seeley, Hadi Afshari, Madalina Furis, Lloyd Bumm

University of Oklahoma

11:00 – 11:20 (A30) Mie-resonator nanofluid for solar thermal applications

Ali K. Kalkan, Ethan Biedenstein, Prabhat Prajapati,

Niloofar, Fatemipayam, Joshua D. Ramsey, and Fardin Mahatab

Oklahoma State University

11:20 – 11:40 (A33) Exploring the phonon band structure of organic optoelectronic

molecular materials

Michael A. Walkup, Lloyd A. Bumm

University of Oklahoma

11:40 – 12:00 (A34) Enhancing multifunctional utility by nanoparticles dispersion in

Kevlar for advanced materials applications

Darshani H. D. DewageDona, Oluwafemi P. Akinmolayan, Isaac Carney, James

M. Manimala and Frank D. Blum

Oklahoma State University

<u>Session 2 – Biochemistry – Room 102, Global Learning Center</u>

Session Chair: Dr. Sean Kim

10:00-10:20 (A4) Inhibition of HDAC1 Using a New Hydroxamate Compound

Kong K Lee, Sean Kim

Northeastern State University

10:20-10:40 (A5) Apigenin Induces Apoptosis in MDA-MB231 Cells In Vitro

Joel Gaikwad, Jayme James, Jonathan Gaikwad and Janaki Iyer

Oral Roberts University, Northeastern State University

10:40-11:00 (A6)

Design, Synthesis, and Evaluation of a Novel Histone Deacetylase
Inhibitor for Cancer Therapy
Nicol L. Nightingale, Sean Kim
Northeastern State University

11:00-11:20 (A7)

Analyzing the effect of allicin on the viability of triple-negative breast cancer cells
Theodore N Quarcoopome, Jonathan Gaikwad, Joel S Gaikwad
Oral Roberts University

11:20-11:40 (A8) Aspirin Analogs as Potential HDAC Inhibitors

<u>Baljit Sandhar</u>, Sean Kim Northeastern State University

Session 3 - Organic - Room 101, Global Learning Center

Session Chair: Dr. Angus Lamar

10:00-10:20 (A13) Metal-free C-H Bond Amination Reactions for the Synthesis of Fused

Tricyclic Heteroarenes

Jeanne L. Bolliger

Oklahoma State University

10:20-10:40 (A14) Halogen-Bonding Photocatalysis Using Carbazole-Based Electron

Donor Catalysts

<u>Negin Shafiei</u>, Dr. Spencer Pitre *Oklahoma State University*

10:40-11:00 (A15) Halocyclopropanation of olefins promoted by nucleophilic cobalt

photocatalysis

John Hayford G. Teye-Kau, Spencer P. Pitre

Oklahoma State University

11:00-11:20 (A16) Sulfonamide Insertion via N-Centered Radical Chemistry for

Synthesis of Compounds with Anticancer Activity

Angus A. Lamar

The University of Tulsa

11:20-11:40 (A18) Investigation of Cobalt(II) Complexes for Photocatalyzed Reactions

Under Visible Light Irradiation

Subrata Pal, Spencer Pitre Oklahoma State University

11:40-12:00 (A31) Harnessing Carbenes/Nitrenes for Drug Discovery

Indrajeet Sharma

University of Oklahoma

<u>Session 4 – Materials/Polymer – Room 103, Global Learning Center</u>

Session Chair: Dr. Hannah King

10:00-10:20 (<u>C1</u>)	Structural composites from post-consumer poly(ethylene terephthalate) (PET) carpet with recycled polypropylene (PP) resin Liyaqat Ali Kamran, Mohamadreza Y. Azarfam, Aditya Nayar, Frank D. Blum, Ranji Vaidyanathan, Hadi Noori Oklahoma State University
10:20-10:40 (<u>C2</u>)	An Investigation of High Temperature Reactions Between Titanium, Silicon, and Yttrium Oxides Hunter Allen, Dr. Dwight Myers East Central University
10:40-11:00 (<u>C3</u>)	NIR-II Photothermal Conversion by using Organic Cocrystals Yuanning Feng University of Oklahoma

Resham Lal Shrestha

Oklahoma State University

Mesoporous Silica Beads

<u>Session 5 – Inorganic/Physical/Analytical – Room 101, Global Learning Center</u>

The University of Tulsa

Session Chair: Dr. Gabriel LeBlanc

11:00-11:20 (<u>C8</u>)

2:00-2:20 (<u>A9</u>)	Efforts Towards Green Chemistry with a Greenhouse Gas: Synthetic Utilization of Nitrous Oxide Deacon A Herndon, Surya Pratap Singh, Upasana Chatterjee, Kenneth M. Nicholas and Indrajeet Sharma University of Oklahoma
2:20-2:40 (<u>A10</u>)	Mg2+/Al3+ Layered Double Hydroxide Synthesis for Phosphate and Nitrate Removal from Water <u>Patrick D. Kitzel</u> Oklahoma State University
2:40-3:00 (<u>A11</u>)	Curcumin: A model to teach undergraduate chemistry concepts Srimal Garusinghe, Madeline Schutts, Natalie Gaskill, Emma E. Frazier Southeastern Oklahoma State University
3:00-3:20 (<u>A12</u>)	Rapid Fabrication of Nickel-Based Electrodes for Electrochemical Applications Gabriel LeBlanc

3:20-3:40 (A17) Evolution of Black Carbon upon Coating with Biomass Burning Organic Aerosol: Interactions at the Wildland-Urban Interface

Christian A. Escritt, Katrina L. Raincrow, Micah R. Miles, Elijah G.

Schnitzler

Oklahoma State University

Session 6 - Physical/Materials - Room 103, Global Learning Center

Session Chair: Dr. Frank Blum

2:00-2:20 (A26) Adaptation of mechanical exfoliation techniques to the production of

ultra-thin crystalline flakes of organic semiconductors

Lucas F Seeley, Steven M Raybould, Aiden J Guild, Lloyd A Bumm

The University of Oklahoma

2:20-2:40 (A27) Catalytic Transformation of Azide-Modified Gold Nanoparticles via

Visible Light Activation for Biomedical Applications

Mohadeseh Naderi, Shoukath Sulthana, Niloofar Valizadeh Dana, Koie

Kebert, Jimmie Weaver, Yolanda Vasquez*

Oklahoma State University

2:40-3:00 (A28) Post consumer poly(ethylene terephthalate) carpet and recycled mixed

polyolefin resin composites

Aditya Satish Nayar, Anuj Maheshwari, Liyaqat Ali Kamran, Frank D. Blum,

Ranji Vaidyanathan, and Hadi Noori

Oklahoma State University

3:00-3:20 (A29) Reactive Uptake of Ozone onto Secondary Brown Carbon from Catechol in

Thin Films: Kinetics Experiments and Multilayer Modeling

Sithumi M. Liyanage, Meredith Schervish, Habeeb H. Al-Mashala,

Katrina L. Betz, Manabu Shiraiwa, and Elijah G. Schnitzler

Oklahoma State University

<u>Session 7 – Organic – Room 102, Global Learning Center</u>

Session Chair: Dr. Jeanne Bolliger

2:00-2:20 (A19) Allylic Alcohol Activation and Sulfonamidation via Acid-Loaded

Silica Gel Catalysis

Zachary C. Brandeburg, Angus A. Lamar

The University of Tulsa

2:20-2:40 (A20) Synthesis of Selenium-Containing Fused Heterocycles

Susila Thapa, Jeanne L. Bolliger

Oklahoma State University

2:40-3:00 (A21) Synthesis of Enamino Carbonyl Compounds By Ball Milling: A Mechanochemical Synthesis Approach Maghawe Ndlovu, Sved R. Hussaini The University of Tulsa Synthesis of tricyclic and tetracyclic imidazole-containing 3:00-3:20 (A22) heteroarenes Nishan Khanal, Jeanne L. Bolliger Oklahoma State University Late-stage functionalization of N-heterocycles with Sulfenyl-3:20-3:40 (A23) carbenes/nitrenes Prakash Kafle University of Oklahoma Session 8 - Biochemistry/Medicinal - Room 203, Global Learning Center Session Chair: Dr. Odilia Osakwe 2:00-2:20 (C4) A Physical Approach to Protein Folding Pranav Domakonda, Kidthusan Birendra Oklahoma School of Science and Mathematics **Characterization of an insect Pheromone Binding Protein:** 2:20-2:40 (C5) **Implications for Environmentally Friendly Pest Management** Pratikshya Paudel, Omar Al Danoon, Shine Ayyappan, Smita Mohanty Oklahoma State University The Evolution of Cancer Treatment: How Antibody-Drug Conjugates 2:40-3:00 (C6) **Are Changing Oncology** Christina L. Dang and Julianne N. Hoang Oklahoma School of Science and Mathematics Harnessing Mycoestrogens: Investigating Phallus impudicus for 3:00-3:20 (C7) **Estrogen Receptor-Positive Breast Cancer** Anna E. Wilson, Dr. William P. Ranahan Oral Roberts University **Understanding and Managing Cholesterol Profiles: A Comprehensive** 3:00-3:20 (C9) Analysis of LDL and HDL Cholesterol Management Eunice S Kim, Fazlur Rahman

Oklahoma School Of Science and Mathematics

B21. Fe(OTf)3 or Blue Light Activated Diazo-Thioglycoside Donors for Glycosylations Umesh Chaudhary, Adrienne Daróczi

The University of Oklahoma

B22. Optimization of reaction conditions for nucleophilic addition to 6-bromo-1,1-dichloronaphthalen-2-one

<u>Audrey A. Iskandar</u>, Steven G. Stagg, Angus A. Lamar *The University of Tulsa*

B23. Domino Synthesis of 1,2,3,5-Tetrasubstituted 1H-Indoles

<u>Siddhartha Maji</u>, Kwabena Fobi, Ebenezer Ametsetor and Richard A. Bunce *Oklahoma State University*

B24. Selective N-alkylation of 1,2,4-triazoles and imidazoles

McKenzie L. Menefee, Jeanne L. Bolliger Oklahoma State University

B25. Cross-electrophile coupling mediated by nucleophilic cobalt photocatalysis

Aishwarya Satish Nayar Oklahoma State University

B26. Benzo[d]oxazoles from Anilides by N-Deprotonation-O-SNAr Cyclization

<u>Nash E. Nevels</u>, Luke Subera, and Richard A. Bunce *Oklahoma State University*

B27. Mechanistic study in new synthetic methods of N-alkenyl 1,2,4-triazolones and 1,3-imidazolones

<u>Abigail C. Norris</u>, Jeanne L. Bolliger *Oklahoma State University*

B28. Bromination of Indazole and Pyrazole Derivatives via Organocatalytic Activation of N-Bromosuccinimide

<u>Muhammad Qasid</u>, Angus A. Lamar *The University of Tulsa*

B29. Alkoxy Substituent Variation of Ethyl

4-((4-methoxybenzyl)thio)-3-(4H-1,2,4-triazol-4-yl)benzoic Acid Kaitlyn M. O'Brien, Jeanne L. Bolliger

Oklahoma State University

B30. Biomolecule Conjugation to Dye-Doped Silica Nanoparticles

<u>Brandi P Woods</u>, Nathan S Green *Northeastern State University*

B31. Vitamin B_{12} Electrochemistry Using Electrodes

<u>Paige M Robertson</u>, Subrata Pal *Oklahoma State University*

B32. Two-Step Synthesis of 1,2,4-Trisubstituted Naphthalene Analogs

<u>Steven G. Stagg</u>, Audrey A. Iskandar, Angus A. Lamar *The University of Tulsa*

B33. Synthesis of 4-(tert-butyl) Pyridine from DHP and 4-Cyanopyridine Utilizing Photo Mediated Redox Processes

<u>Kayman B. Ross</u>, Viraj K. Arachchige, and Spencer P. Pitre *Oklahoma State University*

B34. Study of iodine distribution and concentrations in western Oklahoma brine waters and recycling of used chloroform

Amanda Lane, Alaina Pierce, Jason R. Wickham, Averie Larson, Josena Frame, Kathryn Baugh, and David Edlin Northwestern Oklahoma State University

B35. Halogen-Bonding Photocatalysis Using Carbazoles as Electron Donors

<u>Samuel J Scovitch</u>, Tarannum Tasnim, Negin Shafiei, and Spencer P. Pitre *Oklahoma State University*

B36. Assessing Forever Chemical Contamination in Northeastern Oklahoma Using LC MS/MS

<u>Baboucarr Awe</u>, Foysal Md. Hasan, Ismail Erfan, and Kenneth Roberts *The University of Tulsa*

B37. Generation of Light-Absorbing Carbonaceous Aerosol from Thermal Degradation of Plastics and Whitening through Atmospheric Irradiation

Asma Soofi, Elijah Schnitzler Oklahoma State University

B38. Temporal analysis of Kiamichi river water quality using mollusk bioindicators

Erfan Smiley and Dr. Kenneth Roberts

The University of Tulsa

B39. DOM in Oklahoma Waters

<u>Colter I Bufford</u>, Shawna York <u>Southern Nazarene University</u>

B45. Electrochemical Measurement of Freeze-Thaw Cycle Impact on Sarcoplasmic Oxidation in Beef

<u>Silan Bhandari</u>, Sachinthani A. Devage, Rishav Kumar, Dr. Ranjith Ramanathan, and Dr. Sadagopan Krishnan *Oklahoma State University*

B46. Non-Enzymatic Glucose Detection using Spray Painted Electrodes from 3D Printed Masks

Ashlyn Stephenson and Gabriel LeBlanc

The University of Tulsa

B47. Sensitive and selective label-free capacitance sensor for infectious biomolecule detection

<u>Sathya Samaraweera</u>, Joshua D. Ramsey, and Sadagopan Krishnan *Oklahoma State University*

B48. Spatiotemporal Assessment of Trace Metal Contamination in the Kiamichi River, Oklahoma

Md Foysal Hasan, Lauren Haygood, Baboucarr Awe, Erfan Smiley, and

Kenneth Roberts *The University of Tulsa*

B49. The Chemistry of Artificial Sweeteners

Arastu Manral and Andrew Wang

Oklahoma School of Science and Mathematics

B50. Meat Science: Determining the species-specific heme protein redox behavior using an electrochemical approach

Sachinthani U.K Ayabadda Devage, Silan Bhandari, Minha Arankuny,

Ranjith Ramanathan, and Sadagopan Krishnan

Oklahoma State University

B51. Electrodeposition of Metal Oxides for Use in Perovskite-Based Solar Cells

<u>McCaleb L Doyle,</u> Ethan Falconetti, Julian Talmon, and Gabriel LeBlanc *University of Tulsa*

B57. Introducing Simpler Chemistry- A New Approach

Odilia N Osakwe

Tulsa Community College

B58. Electrodeposition of Catalytic Platinum on 3D Printed Nickel Electrodes

Chetna Mandurai and Gabriel LeBlanc

University of Tulsa

B60. Electrodeposition of ZnO on Plastic-Based Substrates for Solar Cell Applications

Maivi Nguyen and Gabriel LeBlanc

University of Tulsa

B61. Computational and Experimental Study of Amine-Based Sorbent for CO2 capture at low Pressure

Aaron T. Caesar and Nicholas F. Materer

Oklahoma State University

B62. Cost-Effective Fabrication of Ag/AgCl Reference Electrodes for Electrochemical Applications

Abigail Ott and Gabriel LeBlanc *University of Tulsa*

B63. Colorimetric Hybridization sensor mechanism for multiple target detections

<u>Colton J. Scott</u> and Aubri West *Oklahoma State University*

<u>B64</u>. Evaluation of Affordable Systems for Electrochemical Research

<u>Julio C Suarez</u>, Rachel Lewis, and Gabriel LeBlanc *University of Tulsa*

B65. Green Synthesis of Silver Nanoparticles from Aqueous Clove Extract and their Antioxidant Activity

Quentin Woodson and Deshani Fernando Mid-America Christian University

B66. 3D-Printed Electrodes Coated with Nickel Spray Paint for Hydrogen Gas Generation

Rachel M Lewis and Gabriel LeBlanc *University of Tulsa*

B67. Catalytic Transformation of Azide-Modified Gold Nanoparticles via Visible Light Activation for Biomedical Applications

<u>Niloofar Valizadeh Dana</u>, Mohadeseh Naderi, Shoukath Sulthana, Koie Kebert, Jimmie Weaver, and Yolanda Vasquez *Oklahoma State University*

Afternoon Poster Session (Abstracts B1-B20; B40-B44; B52-56; B68-73)

2:00-4:00

B1. An Insight into the Mechanism of Ostrinia furnacalis Pheromone Binding Protein 2: Mutagenesis, Expression and Purification

Ahmad Tijani Azeez and Smita Mohanty Oklahoma State University

B2. Bioactivity Assessment of a Metabolic Inhibitor from Parsley Essential Oil in Lung Cancer Cells

Adeleye A. Edema and Robert J. Sheaff *The University of Tulsa*

B3. Expression and Purification of TMPRSS2

Patrick B Combs

Oklahoma State University

B4. Inhibition of Histone Deacetylases by a Novel Synthetic Hydroxamic Acid Compound

<u>Connor Ferlazzo</u> and Sean Kim Northeastern State University

B5. Glycosylation Enrichment Characterization of Full Length Human γ-sarcoglycan

Jonas G. Ewusi and Michael S. Harris

Oklahoma State University

B6. High Throughput Screening and Docking to Find an Effective Inhibitor to M11 Protein

Benjamin Wu and Delwar Hossain Oklahoma School of Science and Mathematics

B7. Recombinant Expression and Purification of Two Ectodomains of Syndecan-1

Wai Phyo Than (Norman) and Gabriel A. Cook

Oklahoma State University

B8. Design and Characterization of Bio-Based Polyurethane Adhesives Utilizing Schiff Base Diols as Crosslinkers

<u>Yashkumar N. Patel</u>, Rutu Patel, Mayankkumar L. Chaudhary, and Ram K. Gupta *Pittsburg State University*

B9. The Inhibition of a Metallo Beta-Lactamase from Klebsiella pneumoniae by a Salicyl Alcohol-containing Compound

Lydia E. Neff and Sean Kim Northeastern State University

B10. Temperature Dependence of Light-Absorbing Charge-Transfer Complexes in Components of Biomass Burning Organic Aerosol

<u>Holly B. Anthony</u>, Colton T. Calvert, and Elijah G. Schnitzler *Oklahoma State University*

B11. M (Mn/Fe/Co/Ni)-N-C Catalysts for Versatile Electrochemical Applications

<u>Kemilaben Chaudhary</u>, Harsh Panchal, Ronit Chaudhari, and Ram K. Gupta *Pittsburg State University*

B12. Characterization and Biochemical Analysis of Bacteriophage Eastview9101

<u>Gokul Maniventhan</u> and Ismael Leon <u>Southeastern Oklahoma State University</u>

B13. Inhibitory Effect of Histone Deacetylase 8 by a Hydroxamic Acid Compound

<u>Evann Walker</u> and Sean Kim Northeastern State University

B14. Expanding the Pulay SQM Method to Modern Split Valence Basis Sets

John R. McLaughlin, Juhyeon Moon, and William B. Collier *Oral Roberts University*

B15. Synthesis of Histone Deacetylase (HDAC) Inhibitor Analogs Towards Gold Nanorod Surface Coatings

<u>Charli Woessner</u>, Nathan Green, and Sean Kim *Northeastern State University*

B17. Biobased Polyesters Derived from 1,4-Butanediol and a Variety of Aliphatic Diacids

<u>Vinash Chaudhari</u>, Pranabesh Sahu, and Ram K. Gupta *Pittsburg State University*

B18. Performance of a DFT cluster-continuum model for predicting redox potentials of oxvanions in aqueous solution

<u>Aneeq Ahmed</u>, Cora Brown, and Gordon H. Purser *University of Tulsa*

B19. Advanced Bio-Based Polyurethane Coatings: Optimizing Strength and Hydrophobic Properties

<u>Kinal Chaudhari</u>, Mayankkumar L. Chaudhary, Rutu Patel, and Ram K. Gupta *Pittsburg State University*

B20. Evolution of Carbonaceous Aerosol from the Thermal Degradation of Plastics through Atmospheric Oxidation: From Filter-Deposited to Airborne Particles

Micah R. Miles, Katrina Betz, and Elijah J. Schnitzler Oklahoma State University Department of Chemistry

B42. Bio-Based Thermosets: Influence of Various Diols and Diisocyanates

<u>Mayankkumar L. Chaudhary</u>, Rutu Patel, and Ram K. Gupta *Pittsburg State University*

<u>B40</u>. Comparative Analysis of Green Synthesized Silver Nanoparticles from *Citrus limon*, *Citrus reticulata*, and *Citrus sinensis* Fruit Peel Extracts

<u>Isabel Ray</u>, Gershom Smith, Stormy Haynes, and Deshani Fernando *Mid-America Christian University*

B41. Influence of Crosslinkers on the Mechanical and Thermal Characteristics of Bio-Based Polyurethane Adhesives

<u>Jaymin Joshi</u>, Mayankkumar L. Chaudhary, Rutu Patel, and Ram K. Gupta *Pittsburg State University*

B44. Core-Shell Silica Nanoparticle Synthesis and Surface Functionalization

Brenna K.Y. Maynard and Nathan S. Green

Northeastern State University

B52. Bio-Based Adhesives: The Role of Diamine and Triamine Cross-Linkers in Soybean Oil-Derived Non-Isocyanate Polyurethane

Sauravkumar Patel, Chandan Bodhak, and Ram K. Gupta *Pittsburg State University*

B53. Transistor Technology: Fast, Present & Future

Bishal Lamichhane and Delwar Hossain

Oklahoma School of Science and Mathematics

B54. Two-stage Transesterification and Melt Polycondensation for the Synthesis and Characterization of Bio-Based Aliphatic Polyesters

<u>Rutu Patel</u>, Mayankkumar L. Chaudhary, and Ram K. Gupta *Pittsburg State University*

Efforts Towards the Development of a Synthetic Pathway for Catenulobactin B and Its Analogs: A Step Forward for Novel Antibiotic Delivery Systems

<u>Theodore N Quarcoopome</u>, Arielle Whitner, and Prathibha Desman Patel Oral Roberts University

B56. Developing FeCo-NC alloy for optimizing electrocatalytic activity in water splitting and oxygen reduction

<u>Harsh Panchal</u>, Ronit Chaudhari, Kemilaben Chaudhary, and Ram K. Gupta *Pittsburg State University*

B68. In Silico and Enzyme Kinetic Evaluation of HMP-Alkyne as a Metallo-β-Lactamase Inhibitor

Houa Thao and Sean Kim

Northeastern State University

B69. Composition of Carbonaceous Aerosol from the Thermal Degradation of Plastics and Comparison to the Bulk Materials Using ATR-FTIR Spectroscopy

<u>Jace A. Barton</u>, Asma Soofi, and Elijah Schnitzler *Oklahoma State University*

B70. Fe(OTf)3 or Blue Light Activated Diazo-Thioglycoside Donors for Stereoselective Glycosylations

<u>Adrienne Daroczi</u>, Umesh Chaudhary, and Surya Pratap Singh *University of Oklahoma*

B71. Artificial Photosynthesis and Recent Developments

Shantipriya Awasthi, Steven Otzoy, and Fazlur Rahman

B72. Exploring Diphosphadisilatetrahedranes as Precursors for a Novel Zintl Anion

JP Sanza, and Mira Kessler Oklahoma State University

B73. Combining Anharmonic Corrections with SQM Pulay Style Scale Factors to Improve Molecular Vibration Predictions

<u>JuHyeon Moon</u>, and William B. Collier *Oral Roberts University*

ABSTRACTS

A1. Au Magic Fingers in Air: Solvent-Driven Nanostructure Formation on Au(111)

<u>Nazila Hamid</u>, Dillon Dodge, Rowan Dirks, Lauren F. Hornbrook, Erin V. Iski *The University of Tulsa*

The formation of Au magic fingers on Au(111), first observed under "pristine" ultra-high vacuum (UHV), has intrigued researchers for its implications in nanoscale manipulation and quantum effects. This study demonstrates their reproducible formation under ambient conditions (in air, at room temperature) using Scanning Tunneling Microscopy (STM), highlighting the role of solvent chemistry and tip-surface interactions. Exposure of Au(111) to 0.1 M solvent solutions revealed three surface disturbance categories: significant & organized (SOD), significant & disorganized (SDD), and insignificant (IND). SOD, exemplified by Au magic fingers, was most pronounced with solvents like HClO4 and HNO3, which possess high electronegativity and strong electrolytic behavior, facilitating Au atom mass transport. Solvents with electronegative atoms (e.g., HCl) weakened Au-Au bonds, forming thicker nanostructures, while others (e.g., CHCl3) showed minimal disturbance. This work advances the understanding of solvent-surface interactions and demonstrates ambient STM's potential for nanoscale manipulation, enabling applications in nanotechnology, catalysis, and surface chemistry without UHV or liquid layers.

A2. Catalytically Relevant Charge Transfer Reactions at Metal-Organic Framework-Liquid Interfaces

<u>Hyunho Noh</u>, N. Gökçe Altınçekiç, Hafsa Abdul Ghuffar, Chance W. Lander, Zachary J. Ingram, Miguel A Liuzzi-Vaamonde, Anne Martin Salazar. *University of Oklahoma*

H-atom transfer (HAT) and O-atom transfer (OAT) reactions at solid-liquid interfaces are fundamental to modern-day energy and chemical sectors. In these reactions, the binding energies of H/O-atoms at a catalyst surface govern overall reactivity and selectivity. The structural ambiguity and complexity of the catalyst surface preclude a fundamental understanding of these catalytically relevant thermodynamics and kinetics with atomic-level structural precision. Here, we present our recent efforts in measuring the thermodynamics and kinetics of HAT/OAT

reactions using structurally well-defined metal—organic frameworks (MOFs). We first describe our studies electrochemically and computationally measuring HAT thermodynamics using redox-active MOFs with Ti-oxo and Ce-oxo clusters. Then, we describe our more recent work describing structure-activity relationships of Lewis acidic Zr-based MOFs on OAT reactions. Implications of these measurements in heterogeneous catalysis will be discussed.

A3. Mechanical Exfoliation and Optoelectronic Characterizations of 1,4,8,11,15,18,22,25-octabutoxyphthalocyanine Thin Films

<u>Steven M. Raybould</u>, Lucas Seeley, Hadi Afshari, Madalina Furis, Lloyd Bumm. *University of Oklahoma*

Solution-processed organic thin films (OTFs) have emerged as a promising material for optoelectronics applications and exploration due to their wide array of properties including tunability, optical transparency, electrical conductivity and mechanical flexibility. Here, we present our work on 1,4,8,11,15,18,22,25-octabutoxyphthalocyanine (H2OBPc) OTFs, an organic semiconductor that is solution-processable, creating crystalline structures which exhibit high optical anisotropy. Mechanically, the crystals are also anisotropic, the molecules are arranged in layers, held together by moderate strength pi-pi forces, with much weaker (102-103 times) interlayer van der Waals forces, making them analogous to conventional 2D layered materials (2DLMs). We applied a 2DLMs exfoliation procedure on hollow-pen written H2OBPc OTFs to obtain single-crystal flakes with thicknesses on the order of 10-100 nm. Polarized light microscopy was used to confirm the crystallinity of the exfoliated flakes. Atomic force microscopy and its variants were used to measure the thicknesses of the exfoliated flakes and explore their optoelectronic properties.

A4. Inhibition of HDAC1 Using a New Hydroxamate Compound

Kong K Lee, Sean Kim Northeastern State University

Histone deacetylases (HDACs) represent a pivotal group of proteins governing the deacetylation of lysine residues on histones, thereby regulating gene expression. The impact of HDAC activity involves the suppression of genes, including those encoding tumor suppression factors. This makes HDAC a promising target for therapeutic intervention against cancer. Our investigation focuses on HDAC1, a member of Class I HDACs containing a zinc ion in the active site. To identify a potent inhibitor for HDAC1, we synthesized N-[6-(Hydroxyamino)-6-oxohexyl] benzamide, which contains a zinc-binding group, hydroxamate. Our methodology commenced with the synthesis of the hydroxamate compound, and its identification was supported through Thin Layer Chromatography and Nuclear Magnetic Resonance. Additionally, the inhibitory potency was evaluated using an IC50 assay, revealing a value of 5.6 μ M. The Δ G value was calculated to be -9.9 kcal/mol. The overall approach of this research contributes to vital insights into the development of targeting HDACs.

A5. Apigenin Induces Apoptosis in MDA-MB231 Cells In Vitro

<u>Joel Gaikwad</u>, Jayme James, Jonathan Gaikwad and Janaki Iyer *Oral Roberts University, Northeastern State University*

Breast cancer is the most prevalent malignancy among women, with an estimated 264,000 new cases diagnosed annually (Basic Information About Breast Cancer, 2022). The escalating incidence of this disease underscores the critical need for novel therapeutic approaches. This study employed the MDA-MB-231 breast cancer cell line to investigate the apoptotic potential of apigenin, a plant-derived flavonoid with recognized therapeutic properties. Results from MTT assays demonstrated a dose-dependent induction of apoptosis by apigenin. Furthermore, Caspase-3 assays confirmed apigenin-mediated cell death through activation of the caspase pathway. Flow cytometry analysis revealed that apigenin downregulated PDL-1 expression in MDA-MB-231 cells.

A6. Design, Synthesis, and Evaluation of a Novel Histone Deacetylase Inhibitor Cancer Therapy

Nicol L. Nightingale, Sean Kim Northeastern State University

Histone deacetylase inhibitors (HDACi), like suberoylanilide hydroxamic acid (SAHA), show promise in reducing cancer growth by returning apoptotic tumor suppression functions to cancer cells but face selectivity issues that lead to debilitating side effects. An analog of SAHA was designed using Pymol and molecular docking simulations using AutoDock Vina software predicted N-[6-(hydroxyamino)-6-oxyhexyl]benzamide would have a strong binding affinity for the HDAC active-site zinc ion. Synthesis confirmed by TLC, HNMR, and IR analyses led to inhibition studies, revealing an IC50 of 8.9 μ M for HDAC1. SAHA demonstrated significantly greater cytotoxicity than the inhibitor in Vero cells, indicating a broad-spectrum effect, while the inhibitor's cytotoxicity remained selective for A549 cells. The observed time-dependent effects suggest that prolonged exposure enhances the cytotoxic potential of both compounds. However, further studies are required to understand its physiological behavior and potential effectiveness as a therapeutic drug.

A7. Analyzing the effect of allicin on the viability of triple-negative breast cancer cells

<u>Theodore N Quarcoopome</u>, Jonathan Gaikwad, Joel S Gaikwad *Oral Roberts University*

Breast cancer is one of the most prevalent types of cancer among females and a leading cause of cancer-related deaths worldwide. While early detection and treatment can lead to favorable prognoses, the need for highly effective treatments with minimal side effects persists. Allicin, an organosulfur compound found in garlic (Allium sativum), was tested on MDA-MB-231 cells, a highly aggressive triple-negative breast cancer cell line, for evidence of selective cytotoxic activity. Initial microscopic observation suggested induction of apoptosis. Preliminary assay data indicated a decrease in cell viability and elevation of caspase-3 activity, further indicative of apoptosis. Current efforts include comparative examination of the effects of allicin on HEK293T

cells and other noncancerous cell lines at various concentrations. Future investigations will explore the effects of allicin on other cancer cell lines and compare its activity to other natural compounds in garlic.

A8. Aspirin Analogs as Potential HDAC Inhibitors

<u>Baljit Sandhar</u>, Sean Kim Northeastern State University

Cancer is a major health challenge characterized by uncontrolled cell proliferation and metastasis, necessitating the development of effective therapeutic strategies. Histone deacetylase (HDAC) inhibitors have emerged as promising anticancer agents by upregulating gene expression, including tumor suppressor genes. However, the adverse side effects associated with current HDAC inhibitors highlight the need for more selective and less toxic alternatives. This study aimed to synthesize and evaluate 2-acetoxybenzoic acid, 3-acetoxybenzoic acid, and 4-acetoxybenzoic acid as potential HDAC inhibitors and assess their viability for cancer treatment based on toxicity profiles. These compounds were designed as meta and para position analogs of aspirin. Their successful synthesis was confirmed through thin-layer chromatography (TLC), proton nuclear magnetic resonance (1H NMR), and infrared (IR) spectroscopy. Future investigations should focus on assessing the inhibitory potential of these compounds across various HDAC isoforms to establish their specificity and efficacy. Additionally, further studies involving diverse cancer cell lines are warranted to validate their cytotoxicity and therapeutic potential.

A9. Efforts Towards Green Chemistry with a Greenhouse Gas: Synthetic Utilization of Nitrous Oxide

<u>Deacon A Herndon</u>, Surya Pratap Singh, Upasana Chatterjee , Kenneth M. Nicholas and Indrajeet Sharma

University of Oklahoma

Nitrous oxide (N2O), colloquially known as laughing gas, is a long-lived greenhouse gas, 300 times more potent than carbon dioxide (CO2). Furthermore, N2O is chemically inert; only a handful of nitrous oxide reactions are known, mostly occurring under harsh conditions and at highly elevated temperatures. Unlike CO2, N2O is kinetically stable and a poor ligand. However, looking at N2O as an organic synthon, it holds potential. N2O contains a nitrogen-to-nitrogen bond with near triple-bond character and a weak nitrogen-to-oxygen bond. From a disconnection point of view, N2O is an oxidizing agent with a thermodynamic driving force as N2 gas is liberated. There are a handful of literature reports where nitrous oxide is used as a selective oxidant. Moreover, the use of N2O as a nitrogen source and its full incorporation (N and O) into reaction products is an unexplored opportunity. Overall, N2O is a historically underexplored reagent in synthetic chemistry that holds untapped potential as a green reagent.

A10. Mg2+/Al3+ Layered Double Hydroxide Synthesis for Phosphate and Nitrate Removal from Water

Patrick D. Kitzel

Oklahoma State University

Urban runoff and common agricultural practices carry plant nutrients, including phosphates and nitrates, into water systems where they are likely to contribute to the formation of algal blooms. Algal blooms cause significant environmental damage and fiscal repercussions. To remedy this, porous sorbent materials that capture and remove phosphates and nitrates from the water can be synthesized as a preventative measure against algal blooms. Potential sorbents were synthesized via a co-precipitation method using a constant 2:1 ratio of divalent Mg2+ and trivalent Al3+ metals against varying ratios of Na2CO3 and NaOH. Additions varied between 0.00 to 0.10 moles of Na2CO3 and between 0.30 to 0.40 moles of NaOH. To simulate the removal of plant nutrients from aqueous environments, uptake measurements using phosphate and nitrate stock solutions of K2HPO4 and KNO3 were performed. Following optimization analysis, adsorption isotherms and material kinetics were explored to further characterize final LDH materials with additional exploration into column studies.

A11. Curcumin: A model to teach undergraduate chemistry concepts

<u>Srimal Garusinghe</u>, Madeline Schutts, Natalie Gaskill, Emma E. Frazier Southeastern Oklahoma State University

General chemistry concepts are the gateway to science majors. However, students demonstrate difficulty remembering concepts and recalling them effectively when needed. The unfamiliarity with the structural formula of molecules was identified as a challenge that first-year students face. Instead of teaching multiple concepts around several molecules, this research study investigates how to teach various undergraduate concepts around a single molecule, curcumin, and how to transform learned concepts for problem-solving. The potential use of curcumin in intermolecular forces, UV-visible spectroscopy, acid-base titrations, and synthesis of metal complexes will be discussed in the presentation.

A12. Rapid Fabrication of Nickel-Based Electrodes for Electrochemical Applications

Gabriel LeBlanc

The University of Tulsa

Electrodes are a fundamental aspect of electrochemical systems. Many commercial electrodes can be expensive, while more cost-effective electrodes can be difficult to prepare for unique experiments. Recently, rapid prototyping tools such as 3D printing have been utilized to generate custom electrodes quickly and inexpensively, though often with high resistance values. Recently we developed an alternative electrode fabrication technique that uses conductive metal paints to convert a wide range of materials into functional electrodes. We are now interested in using these electrodes in a wide range of electrochemical applications including electro-organic synthesis,

hydrogen fuel generation, battery technologies, and sensors. Each of these areas leverages the ability to modify different materials. For example, to increase the active surface of the electrode for more efficient electro-organic synthesis, we use 3D printed materials. For wearable sensor applications, we are exploring how flexible plastic substrates can be used. These demonstrate the versatility of this method, which we hope inspires researchers in a variety of fields.

A13. Metal-free C-H Bond Amination Reactions for the Synthesis of Fused Tricyclic Heteroarenes

Jeanne L. Bolliger *Oklahoma State University*

Heterocycles are of critical importance to the biological activity of many agrochemicals and pharmaceuticals. As such, both the synthesis of new scaffolds and the development of new methodologies for preparing known heterocycles can lead to advances in related fields. The Bolliger group has developed a new strategy to nitrogen-containing tricyclic heteroarenes containing a variety of substituents. Both aromatic and aliphatic N-substituents are tolerated, and the iodine-promoted C–H amination step is compatible with a wide range of functional groups including esters, amides, alcohols, alkynes, and alkenes. Careful reaction monitoring by LCMS and in situ NMR experiments allow us to propose a mechanism for this C–H bond amination reaction yielding fused tricyclic heteroarenes.

A14. Halogen-Bonding Photocatalysis Using Carbazole-Based Electron Donor Catalysts

Negin Shafiei, Dr. Spencer Pitre Oklahoma State University

Halogen-bonding-based charge-transfer complexes have been identified as an alternative for generating carbon radicals, yet there are few reports utilizing (fluoro)alkyl bromides. Here, we present a dual catalytic system for radical formation from α -bromodifluoroesters and amides under visible-light irradiation. Mechanistic studies reveal that in situ bromide displacement by a catalytic iodide salt forms a C–I bond, subsequently activated by our hydroquinone halogen-bonding catalyst. We will share our findings on optimizing the reaction conditions, reaction scope and mechanistic studies. Expanding on our halogen-bonding platform, we recently developed a versatile approach to generate radicals from non-fluorinated alkyl halides using carbazole-based electron donors, which effectively catalyze radical formation through either halogen bonding or a typical photocatalytic pathway under irradiation. Our findings on optimizing reaction conditions, the reaction scope, and mechanistic studies will be presented.

A15. Halocyclopropanation of olefins promoted by nucleophilic cobalt photocatalysis

John Hayford G. Teye-Kau, Spencer P. Pitre Oklahoma State University

The cyclopropane moiety with unique chemical properties is ubiquitous in natural products and important bioactive molecules. These molecules are being explored as candidates for anticancer, antifungal, and other therapeutic applications. In this regard, mono-halogenated cyclopropanes can serve as important building blocks for synthesizing diverse cyclopropane scaffolds. Existing mono-halocyclopropanation strategies employ toxic metal hydride catalysts, lack operational simplicity, and tend to produce unselective mixtures of products, highlighting the need for more efficient, and greener strategies. Employing Vitamin B12 as a nucleophilic cobalt photocatalyst with haloforms as the halo-methylene source, a photo-mediated strategy for the halo-cyclopropanation of electron-rich olefins will be presented. The reaction proceeds via an SN2 route to generate the key dihalomethyl–Co(III) intermediate which undergoes photolysis with visible-light irradiation, affording a dihalomethyl radical which reacts further with olefins to produce the expected halocyclopropanes in good yields with excellent diastereoselectivities, primarily favoring the thermodynamically unfavored cis-1,2-disubstituted cyclopropane.

A16. Sulfonamide Insertion via N-Centered Radical Chemistry for Synthesis of Compounds with Anticancer Activity

Angus A. Lamar The University of Tulsa

Due to the prevalence of sulfonamides in pharmaceuticals, agrochemicals, and advanced materials, the development of atom-economical, operationally simple methods to install these important functionalities remains a valuable goal in the synthesis of fine chemicals. Nitrogen-centered radicals (NCR) have the potential to serve as powerful alternative reagents to traditional carbon-nitrogen (C-N) bond forming methods for the direct transformation of a variety of less accessible chemical functionalities. Historically, NCR reactions have been underexplored relative to analogous carbon radical reactions, largely due to the perceived instability of the reagents and lack of methods for their generation. Our research group has focused on addressing this challenge by developing new visible-light activated reactions that utilize inexpensive materials to generate reactive NCR species from relatively stable, commercially available reagents. Our progress towards the installation of sulfonamide functionality using a NCR precursor to produce molecules with medicinal significance will be presented.

A17. Evolution of Black Carbon upon Coating with Biomass Burning Organic Aerosol: Interactions at the Wildland-Urban Interface

<u>Christian A. Escritt</u>, Katrina L. Raincrow, Micah R. Miles, Elijah G. Schnitzler *Oklahoma State University*

As instances of wildfires increase across the US, the interactions between emissions of biomass burning and urban sources at the wildland-urban interface become more critical to air quality and climate change. In urban environments aggregates of black carbon (BC) are emitted from diesel engines. When biomass burning emissions are transported across the wildland-urban interface, these BC aggregates are exposed to biomass burning organic aerosol (BBOA), composed of many compounds with wide ranges of chemical, physical, and optical properties, including volatility.

The components of BBOA will partition onto the BC aggregates, and the coatings will cause changes to morphology and hygroscopicity of BC, which impact its interactions with radiation and clouds. We investigate the effects of different volatility fractions of BBOA, representative of different ages of plumes with respect to dilution in the atmosphere, on BC restructuring. We determine that, as volatility decreases, more coating is necessary for the same restructuring.

A18. Investigation of Cobalt(II) Complexes for Photocatalyzed Reactions Under Visible Light Irradiation

Subrata Pal, Spencer Pitre Oklahoma State University

Uses of square planar cobalt complexes as photocatalysts are of interest due to their dominant nucleophilic properties in the cobalt(I) oxidation state, which can be leveraged in SN2-type reactions with electrophiles, like alkyl halides. The resulting Co(III)—alkyl intermediate contains a weak Co(III)—C bond that can be photolyzed with visible light irradiation to form radicals. While common commercially available nucleophilic cobalt complexes, such as Vitamin B12, have been adopted as photocatalysts in many C—C bond forming reactions, the investigation of new cobalt complexes that can be used for nucleophilic cobalt photocatalysis remains limited. In this work, we discussed our progress towards the preparation of a series of cobalt(II) complexes and their performance in different photochemical reactions. In particular, the synthesis of a variety of Co(II) complexes and the effects of both the axial and square planar ligands on their catalytic activity are discussed.

A19. Allylic Alcohol Activation and Sulfonamidation via Acid-Loaded Silica Gel Catalysis

Zachary C. Brandeburg, Angus A. Lamar *The University of Tulsa*

Environmentally friendly catalysis has been a focus for decades and has led to multiple developments in supported catalysis. Additionally, recent work in synthetic organic chemistry has illuminated various methods for the activation of allylic alcohols such as with transition metal catalysts and the use of strong acids. Our group has previously demonstrated novel methods for the incorporation of sulfonamide functionality into a variety of structural frameworks such as aromatic and heteroaromatic compounds. This work aims to combine the recent improvements in supported catalysis and allylic alcohol activation along with our group's previous success with sulfonamide synthesis. This new approach allows for a one-pot, environmentally friendly synthesis of allylic sulfonamides under mild conditions, producing only water as the byproduct. Furthermore, the acid-loaded silica gel catalyst is recyclable which is an appealing characteristic in green chemistry.

A20. Synthesis of Selenium-Containing Fused Heterocycles

Susila Thapa, Jeanne L. Bolliger

Oklahoma State University

Heterocycles with one or more heteroelements play an important role in medicinal chemistry. Nowadays, most of drugs contain at least one heterocyclic ring or even fused heterocycles. Recently, several examples of heterocyclic compounds with selenium in the ring, such as selenazofurin and ebselen, have shown promising results in the treatment of various diseases. In this presentation, we will highlight a new synthetic pathway for the preparation of novel tricyclic organoselenium compounds starting from selenium metal. Examples have been selected to demonstrate the wide functional group tolerance of our new synthetic methodology.

A21. Synthesis of Enamino Carbonyl Compounds By Ball Milling: A Mechanochemical Synthesis Approach

<u>Maqhawe Ndlovu</u>, Syed R. Hussaini *The University of Tulsa*

Enamino carbonyl compounds play a crucial role in organic synthesis, serving as versatile intermediates for the synthesis of bioactive molecules, pharmaceuticals, catalytic ligands. Their unique conjugated system, consisting of an amine, alkene, and carbonyl group, provides both nucleophilic and electrophilic sites, making them valuable pharmacophores in drug development. While several synthetic routes to these compounds are available, the continuous search for more efficient and broadly applicable methods remains a vibrant area of research. A prominent approach is the Eschenmoser coupling reaction, which forms enamino carbonyls by reacting a thioamide with an α -halo carbonyl compound in the presence of a base. Despite its effectiveness and substrate tolerance, this method often suffers from lengthy reaction times and limitations with primary thioamides, which tend to form nitriles. Our research explores how mechanochemical techniques, specifically ball milling, enhance this coupling under heterogeneous conditions, improving reaction efficiency and enabling the successful use of primary thioamides.

A22. Synthesis of tricyclic and tetracyclic imidazole-containing heteroarenes

Nishan Khanal, Jeanne L. Bolliger Oklahoma State University

Nitrogen and sulfur-containing fused heterocycles are known to exhibit a range of biological activity. Among them, imidazole-containing compounds are well represented in approved drugs and drug candidates. Using a new cyclization methodology developed in the Bolliger lab, we have demonstrated its utility in the preparation of tricyclic and tetracyclic imidazolium-containing heteroarenes. Our method offers a wide functional group tolerance in combination with reaction conditions tolerant to the presence of air and water.

A23. Late-stage functionalization of N-heterocycles with Sulfenyl- carbenes/nitrenes

Prakash Kafle

University of Oklahoma

Nitrogen-containing heterocycles are ubiquitous in commercial drugs, making their selective modification a key strategy for expanding chemical diversity in drug discovery libraries. Here, we introduce efficient skeletal editing methods leveraging the unique reactivity of sulfenylcarbenes and sulfenylnitrenes to insert single carbon or nitrogen atoms. These transformations enable the conversion of pyrroles, indoles, and imidazoles into challenging scaffolds such as pyridines, pyrimidines, quinolines, quinazolines, and triazines. Notably, sulfenylcarbenes exhibit inverse chemoselectivity compared to conventional carbenes, selectively targeting alkenes while tolerating reactive groups like alcohols, carboxylic acids, and amines. Sulfenyl nitrenes, generated thermally across a broad temperature range (–30 to 150 °C), further expand the scope to oxidation-sensitive functionalities, including phenols and thioethers. These versatile methodologies have been applied to complex natural products, amino acids, and pharmaceuticals. Mechanistic insights and regioselectivity outcomes, supported by DFT calculations, highlight the potential of sulfenyl-carbenes/-nitrenes for precise molecular framework modification.

A26. Adaptation of mechanical exfoliation techniques to the production of ultra-thin crystalline flakes of organic semiconductors

<u>Lucas F Seeley</u>, Steven M Raybould, Aiden J Guild, Lloyd A Bumm *The University of Oklahoma*

Material properties have been shown to dramatically change as the dimensionality of the system decreases, but constraining a system to two-dimensions during synthesis is not possible for all materials. Mechanical exfoliation is a proven low-cost, quick method that can separate a few monolayers of material from a bulk sample, but the applicability of this method to organic systems has thus far been limited. To investigate the thickness dependent excitonic properties of 1,4,8,11,15,18,22,25-octabutoxyphthalocyanine (H2OBPc), we have developed a polydimethylsiloxane (PDMS) based mechanical exfoliation technique which binds to the sample surface via van der Waals forces and polymer adhesion properties. This process leaves no optically visible residue on the thin monocrystalline exfoliated flakes and allows immediate further characterization. Through polarized light and atomic force microscopy methods, the relationship between the crystal structure of bulk films and the mechanism of exfoliation can be understood and translated into marked improvements in flake yield.

A27. Catalytic Transformation of Azide-Modified Gold Nanoparticles via Visible Light Activation for Biomedical Applications

Mohadeseh Naderi, Shoukath Sulthana, Niloofar Valizadeh Dana, Koie Kebert, Jimmie Weaver, Yolanda Vasquez*

Oklahoma State University

A novel visible light-mediated photocatalytic bioconjugation strategy was developed to chemically modify azide-functionalized gold nanoparticles (Au-SH-PEG-N₃) using benzocycloheptene (BC7) as a linker. Under blue LED illumination and in the presence of an iridium-based photocatalyst, the activated double bond in BC7 reacts with surface N3 to form a triazoline click product. NMR spectroscopy confirmed triazoline formation after three hours of reaction. During purification, the triazoline ring undergoes air oxidation to generate a more stable triazole ring, as verified by NMR, FTIR, UV-Vis spectroscopy. This photocatalytic strategy overcomes key limitations of traditional click reactions, including copper-induced cytotoxicity, reagent instability in SPAAC, and unwanted side reactions. To explore potential biomedical applications, functionalized Au nanoparticles were tested for cellular uptake and viability in stimulated and unstimulated RAW 264.7 cells. MTT assays showed low cytotoxicity in unstimulated cells but a marked reduction in viability in stimulated cells treated with Au-Folate-BC7 NPs, indicating a possible anti-inflammatory effect.

A28. Post consumer poly(ethylene terephthalate) carpet and recycled mixed polyolefin resin composites

Aditya Satish Nayar, Anuj Maheshwari, Liyaqat Ali Kamran, Frank D. Blum, Ranji Vaidyanathan, and Hadi Noori *Oklahoma State University*

Around 91% of the used carpets end up in landfills. In addition, only 5 percent of the total US plastic waste was recycled in 2021. A technique was developed for producing recycled composites using post-consumer PET carpet and recycled mixed polyolefin resin (PE & PP). Compression molding was carried out by varying parameters like temperature, pressure, time, composition and configurational alignment of the carpet and resin. These factors were considered to optimize the parameters and achieve better mechanical properties of the composite. Differential scanning calorimetry (DSC) and thermal gravimetric analysis (TGA) were used to guide the initial molding conditions for the carpet and resin combination. Mechanical properties of composites were determined using 3-point bend tests. The resulting moldings exhibited good flexural strengths and moduli to be called structural composites. This method is useful as it allows composites to be made from polymers that have different mechanical and crystallization behavior.

A29. Reactive Uptake of Ozone onto Secondary Brown Carbon from Catechol in Thin Films: Kinetics Experiments and Multilayer Modeling

Sithumi M. Liyanage, Meredith Schervish, Habeeb H. Al-Mashala, Katrina L. Betz, Manabu Shiraiwa, and Elijah G. Schnitzler *Oklahoma State University*

Brown carbon (BrC), or light-absorbing organic aerosol, affects climate directly by absorbing and scattering radiation and indirectly by altering cloud formation. The evolution of the optical properties of BrC is governed by multiphase atmospheric processing, particularly through interactions with oxidants, such as ozone. In this study, we investigate the reactivity of secondary BrC from catechol using coated-wall flow-tube experiments, monitoring the loss of ozone from the gas phase over thin films, and kinetic multilayer modeling. The reactive uptake of ozone to

secondary BrC significantly increased when relative humidity (RH) in the flow-tube increased from 0 to 50%, which aligns with the plasticizing effect of water on secondary organic aerosol. At each RH, the reactive uptake of ozone decreased for thin films that had been exposed to UV radiation in a photo-reactor. These findings highlight the crucial role of environmental conditions in regulating BrC aging and climate effects in the atmosphere.

A30. Mie-resonator nanofluid for solar thermal applications

Ali K. Kalkan, Ethan Biedenstein, Prabhat Prajapati, Niloofar, Fatemipayam, Joshua D. Ramsey, and Fardin Mahatab.

Oklahoma State University

Light trapping in subwavelength structures via Mie resonances is an exciting effect inspiring novel technologies for solar energy harvesting. Here, we explore cupric oxide (CuO) dielectric Mie-resonator particles, dispersed in a solvent, as an efficient nanofluid for solar-to-thermal energy conversion. This promise of subwavelength CuO structures is owed to the high refractive index of CuO (>2.3) enabling efficient light trapping, in addition to its direct, dipole-allowed, and narrow band gap (1.2 eV) allowing for strong light absorption in the visible and near-infrared. The Mie-resonant CuO nanoparticles exhibit enhanced Raman scattering and photothermal efficiency over off-resonant (e.g., ~5-micron-size) CuO particles. Based on the analytical Mie solution and dynamic light scattering measurements, we infer the aggregates of the CuO nanoparticles also behave as Mie resonators. A stable solar-thermal nanofluid with 0.1 wt% CuO was developed, and a proof-of-concept distiller for seawater desalination was demonstrated.

A31. Harnessing Carbenes/Nitrenes for Drug Discovery

<u>Indrajeet Sharma</u> *University of Oklahoma*

In recent years, drug discovery has faced a significant challenge: a slowdown in identifying new drugs and rising development costs. A crucial factor contributing to this stagnation is the limited diversity in screening libraries, emphasizing the need to explore uncharted chemical spaces. To address this issue, the Sharma research group focuses on scaffold-hopping to create novel chemical entities from existing frameworks. While this approach has traditionally been pursued through computational methods, scaffold-hopping methods remain underdeveloped. Current scaffold-hopping strategies often rely on harsh conditions, unstable reagents, or oxidants, which restrict their applicability. Our research tackles these challenges using stable, benchtop-compatible carbene and nitrene precursors. These reagents enable site-selective carbon or nitrogen atom insertions, facilitating transformations such as converting pyrroles to pyridines/pyrimidines and to quinolines/quinazolines. Additionally. indoles 15N-sulfenylnitrene allows for the synthesis of isotopically labeled 15N-heterocycles as chemical probes. This work broadens the chemical toolbox for medicinal chemistry and pharmaceutical applications.

A33. Exploring the phonon band structure of organic optoelectronic molecular materials

Michael A. Walkup, Lloyd A. Bumm University of Oklahoma

Organic optoelectronics have garnered attention for their promise as flexible excitonic materials. One potential candidate, 1,4,8,11,15,18,22,25-octabutoxyphthalocyanine (H2OBPc), could find application in photonic energy transport due to its coherent exciton states. To understand the exciton transport of H2OBPc, the phonon modes must be analyzed to identify those significant to intermolecular exciton coupling. Density functional theory (DFT) calculations were performed using the Vienna Ab initio Simulation Package (VASP). The results of phonon dispersion, band structure, and density of states calculations will be discussed. The process to assign the modes and visualize the atomic eigenvectors will also be discussed as well as searching for those modes that significantly contribute to exciton transport.

A34. Enhancing multifunctional utility by nanoparticles dispersion in Kevlar for advanced materials applications

<u>Darshani H. D. DewageDona</u>, Oluwafemi P. Akinmolayan, Isaac Carney, James M. Manimala and Frank D. Blum *Oklahoma State University*

We investigated the chemical characterization of nanoparticles dispersed onto Kevlar fabric using attenuated total reflectance Fourier-transform infrared (ATR-FTIR) spectroscopy and thermogravimetric analysis (TGA). Silica (SiO₂), alumina (Al₂O₃), and zinc oxide (ZnO) nanoparticles were dispersed at varying concentrations to enhance the material's properties. ATR-FTIR confirmed the successful deposition of nanoparticles and provided insights into their interactions with Kevlar's molecular structure. Thermogravimetric analysis (TGA) was used to evaluate the thermal stability and inorganic residue content of the modified fabric. The results demonstrated that silica, alumina, and zinc oxide nanoparticles significantly improved Kevlar's thermal resistance while maintaining its chemical integrity. The integration of these nanoparticles enhances the fabric's structural stability and heat resistance, making it suitable for demanding applications. These findings contribute to the advancement of high-performance materials, particularly in protective gear, aerospace, and other industries requiring enhanced durability, thermal stability, and mechanical resilience.

B1. An Insight into the Mechanism of Ostrinia furnacalis Pheromone Binding Protein 2: Mutagenesis, Expression and Purification

Ahmad Tijani Azeez and Smita Mohanty Oklahoma State University

Ostrinia furnacalis also known as Asian Corn Borer, a lepidopteran moth, is an agricultural pest found across Asia, Australia, Africa, and some regions of the United States. It is responsible for the destruction of over one-third of the total crops and food stored globally. The O. furnacalis pheromone-binding protein 2 (OfurPBP2) located in the male antennae is involved in detecting

female-emitted pheromones, a crucial step in the mating process. The binding of pheromone to OfurPBP2 is the first step in the signaling events where a chemical signal translates into an electrical signal resulting in the behavioral response in the male. Unlike other lepidopteran PBPs, OfurPBP2 contains a His-Arg gate near the binding pocket instead of the usual His-His gate. The histidine gate, as well as the C-terminal gate, is reported to be involved in the ligand release of several well-studied PBPs. The C-terminus of OfurPBP2 has four additional charged residues in stark difference to the well-studied PBPs. To elucidate the structural mechanism underlying pheromone binding and release in this agricultural pest, we have generated several mutants of OfurPBP2for investigation. Research work carried out on these mutants, including recombinant expression, refolding, and purification of these proteins, will be presented.

B2. Bioactivity Assessment of a Metabolic Inhibitor from Parsley Essential Oil in Lung Cancer Cells

Adeleye A. Edema and Robert J. Sheaff *The University of Tulsa*

Parsley (*Petroselinum crispum*) essential oil contains bioactive compounds with potential anticancer properties. This study aimed to isolate and identify the active compound responsible for cytotoxic effects against A549 lung cancer cells. The essential oil was purified using column chromatography, followed by thin-layer chromatography (TLC) and gas chromatography-mass spectrometry (GC-MS) for compound identification. The cytotoxicity of the fractions was assessed using a Cell Titer Glow assay, with 2-deoxyglucose (2DG) and rotenone as metabolic inhibitors. Two purification steps yielded 38.67% and 33.33% fractions, respectively. The fraction from column 2 exhibited 70% inhibition, comparable to 80% rotenone, suggesting its role in ATP depletion and cancer cell death. These findings highlight the potential of parsley-derived compounds as natural anticancer agents and warrant further investigation into their mechanism of action and therapeutic potential.

B3. Expression and Purification of TMPRSS2

Patrick B Combs

Oklahoma State University

Transmembrane protease serine 2 (TMPRSS2) has been determined as a key factor in SARS-CoV-2 cellular infection and is found in high concentrations in membranes of epithelial cells of the lungs, heart, liver, kidneys, and gastrointestinal tract. TMPRSS2 acts as a primer, cleaving the virus at the S1/S2 boundary and S2' of the S2 domain, exposing the fusion peptide of the spike protein. This, in conjugation with viral anchoring to the cellular angiotensin-converting enzyme 2 (ACE2) receptor, induces virus-host membrane fusion. Understanding of TMPRSS2 and its mechanism of cleavage is crucial in finding novel antiviral medications, since TMPRSS2 has also been found to be a primer for virus-host fusion in other diseases such as MERS, SARS, and influenza. Studying TMPRSS2 will allow insight into not just the infection mechanisms of SARS-CoV-2, but other viruses as well. Presented here is the expression and purification of a TMPRSS2 fusion protein in E. coli.

B4. Inhibition of Histone Deacetylases by a Novel Synthetic Hydroxamic Acid

Compound

<u>Connor Ferlazzo</u> and Sean Kim Northeastern State University

Cancer remains a leading cause of death, with histone deacetylase inhibitors (HDACi) used to impede factors contributing to tumor progression. While current inhibitors show promise, they often lack selectivity, leading to adverse side effects. Autodocking results indicated strong binding of N-[6-(hydroxyamino)-6-oxyhexyl]benzamide to HDAC's active-site zinc ion. An inhibition assay against HDAC1 showed an IC50 of 6.3 μ M, demonstrating effective inhibition. A subsequent assay in HeLa cell lysates against multiple HDACs yielded an IC50 of 12.0 μ M. These results confirm the compound's strong affinity for the HDAC zinc ion. However, its physiological effects remain unknown, necessitating further studies to assess its drug potential.

B5. Glycosylation Enrichment Characterization of Full Length Human γ-sarcoglycan

Jonas G. Ewusi and Michael S. Harris Oklahoma State University

Due to its role in maintaining the structural integrity of muscle cell sarcolemma, γ-sarcoglycan, when deficient, or mutated in cells, results in Limb-Girdle Muscular Dystrophy. γ-sarcoglycan is extremely difficult to recombinantly express in the amounts necessary for biochemical characterization due to its hydrophobic nature. As a result, there is a lack of structural, and dynamic information of this protein. We show here the expression of full-length recombinant γ-sarcoglycan in Escherichia coli, its purification using size exclusion chromatography, and the incorporation of the purified protein in detergents and lipids that mimic the natural membrane environment of the protein. It has been suggested that the addition of a sugar molecule to a protein, a process known as glycosylation, has a direct effect on how the protein folds, interacts with other biomolecules, and functions within the proteome. Glycoproteins play key roles in a myriad of biological processes and are estimated to form as high as 50% of human proteins. This makes glycosylation an essential post-translational modification in proteins. in vitro Glycosylation has been performed as a technique to add sugars synthetically to glycoproteins. Our goal is to enrich glycosylated full-length human γ -sarcoglycan and incorporate it into nanodiscs for structural analysis using Nuclear Magnetic Resonance (NMR) Spectroscopy. NMR has been employed extensively in the study of structures of proteins. One sample environment that has been helpful in studying membrane proteins is Nanodiscs which provides a way around this issue. Nanodiscs have sizes that are structurally similar to the cellular membrane, and as such, are a perfect membrane mimetic. Here, we show the successful in vitro glycosylation of full length γ -sarcoglycan in nanodiscs as well as novel methods of making nanodiscs.

B6. High Throughput Screening and Docking to Find an Effective Inhibitor to M11 Protein

High-throughput screening (HTS) is a process in drug discovery that rapidly tests large chemical libraries against a biomolecular target to identify potential drug candidates. On the other hand, molecular docking is a computational technique to predict how well a small molecule (ligand) will bind to a protein target by simulating its interaction within the protein's binding site. Combining HTS and docking enables a powerful *in silico* virtual screening approach where large chemical libraries are computationally docked to a target protein structure to identify potential promising lead compounds. These methods significantly accelerate drug discovery by narrowing the search space for potential hits. This presentation will report our initial results of high throughput screening and docking of sizeable large-scale molecules from molecular data bank libraries to find a potential inhibitor to the M11 protein.

B7. Recombinant Expression and Purification of Two Ectodomains of Syndecan-1

<u>Wai Phyo Than (Norman)</u> and Gabriel A. Cook *Oklahoma State University*

Syndecan-1 (SDC-1) is part of a family of integral cell membrane heparan sulfate proteoglycan proteins known as Syndecans. SDC-1 is involved in inflammatory response, cell to cell signaling, and other important cell functions. Currently, there are very few studies about the structure and dynamics of SDC-1. Significant interactions on the extracellular ectodomain portion of SDC-1 are where our research efforts could be expanded upon. The ectodomains are often shed by common sheddases, known as matrix metalloproteinases (MMPs), due to various stimuli. As a number of various cancer cells have shown increased levels of MMPs and, as a result, increased levels of SDC-1 ectodomain fragments in sera, they could serve as potential biomarkers when evaluating for certain cancers and diseases. In this research, SDC-11-82 and SDC-11-245 ectodomains are expressed in separate E.coli cell lines. The successful expression and purification of the two proteins will be described. Future studies involving the glycosylation of the ectodomains through in vitro glycosylation will also be outlined.

B8. Design and Characterization of Bio-Based Polyurethane Adhesives Utilizing Schiff Base Diols as Crosslinkers

<u>Yashkumar N. Patel</u>, Rutu Patel, Mayankkumar L. Chaudhary, and Ram K. Gupta *Pittsburg State University*

Traditionally, polyurethanes (PUs) are typically synthesized using petroleum-based polyols such as urea or phenol formaldehyde, which are toxic to humans and harmful to the environment. As a result, in recent times, industries have been interested in developing bio-based PUs made of vegetable oil-based polyol and diisocyanate. In this study, PU-based adhesives are synthesized by using soybean oil polyol (SOP) and methylene diphenyl diisocyanate. To get better performance of synthesized PU adhesive schiff-based diols, named as VB and VH, have been introduced into the system as crosslinkers which are derived from butane diamine, hexane diamine, and vanillin. The successful synthesis of PU has been confirmed with Fourier transform infrared spectroscopy (FT-IT) spectra. The tensile strength of adhesive samples was tested on oak wood coupons. For

VB-based adhesive samples, VB-10wt.% has shown the highest tensile strength of 4400 KPa among all the weight percentages (wt.%), whereas for VH-based adhesive samples, The highest tensile strength has been observed for VH-10wt.% (5000 KPa). In both cases, with increasing the wt.% of Schiff base diol, tensile strength is decreased to 3800 KPa and 2900 KPa for VB-15wt.% and VH-15wt.% respectively. Moreover, the synthesized PU adhesive samples are thermally stable which is confirmed with thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) analysis. In addition, gel content and degree of swelling test further reveal the crosslinking efficiency of the PU adhesive materials.

B9. The Inhibition of a Metallo Beta-Lactamase from Klebsiella pneumoniae by a Salicyl Alcohol-containing Compound

<u>Lydia E. Neff</u> and Sean Kim Northeastern State University

A recurring and prominent issue in the field of biomedical research is the existence of antibiotic resistant bacteria. Antibiotics are commonly used to treat bacterial infections, however, over time bacteria has been able to resist certain antibiotics. This has led to a need for more advanced antibiotics which combat these resistant bacterial strains. It has been found that the most effective way to combat this resistance is by combining an antibiotic with an inhibitor. This can increase the overall effectiveness of the antibiotic. One reason for antibiotic resistance is the presence of lactamases that catalyze the hydrolysis of β -lactam antibiotics. The inhibition of a metallo beta-lactamase from Klebsiella pneumoniae by a salicyl alcohol containing compound was tested *in silico* and in vitro using HMP-alkyne. In vitro enzyme inhibition assays, cell viability assays and thin-layer chromatography were performed in order to determine the inhibition values of HMP-alkyne. The reaction was shown to be time-dependent, with a IC50 of .03 mM and a Ki value of .35 mM. This IC50 shows a strong inhibitory potency for HMP-alkyne. In conclusion, through the in vitro studies, HMP-alkyne is an effective inhibitor of metallo beta-lactamase from Klebsiella pneumoniae.

B10. Temperature Dependence of Light-Absorbing Charge-Transfer Complexes in Components of Biomass Burning Organic Aerosol

<u>Holly B. Anthony</u>, Colton T. Calvert, and Elijah G. Schnitzler *Oklahoma State University*

Biomass burning organic aerosol (BBOA) is a significant source of brown carbon (BrC), which is a complex mixture of light-absorbing organic molecules. In the atmosphere, the climate effects of BrC depend on the balance of absorption and scattering. Methoxyphenol compounds are colorless and abundant in biomass burning emissions. When they interact with quinones in the atmosphere, such as 1,4-benzoquinone, they can form charge-transfer complexes and strongly absorb visible light. Here, the temperature dependence of the light absorption of solutions of methoxyphenols and benzoquinone in n-heptane, a proxy of the non-polar phase of BBOA, was explored using UV-vis spectroscopy. The enthalpies of formation for the respective complexes were calculated using the spectra at different temperatures. The temperature dependence of absorbance from methoxyphenol compounds and benzoquinone in n-heptane confirms the role and relevance of

non-covalent interactions in BBOA, leading to highly absorptive charge-transfer complexes that may impact climate.

B11. M (Mn/Fe/Co/Ni)-N-C Catalysts for Versatile Electrochemical Applications

<u>Kemilaben Chaudhary</u>, Harsh Panchal, Ronit Chaudhari, and Ram K. Gupta *Pittsburg State University*

The design and development of atomically dispersed M-N-C catalysts (metal (M) supported on an NC matrix) with high multifunctional electrocatalytic performance is desirable but proved to be very challenging. Herein, we synthesized M-N-C catalysts (M = Fe, Co, Mn, and Ni) using Zn-assisted high temperature treatment and characterized using various techniques. The prepared catalysts were tested for their electrocatalytic performance towards oxygen and hydrogen evolution reaction (OER and HER) as well as oxygen reduction reaction (ORR) in alkaline media. The results indicated that Fe-N-C catalyst showed higher performance towards both the HER ($\eta 10 = 65 \text{ mV/cm2}$) and OER $(\eta 10 = 283 \text{ mV/cm}^2)$ as compared to other prepared catalysts. In contrast, Mn-N-C displayed excellent ORR activity (E1/2 = 0.90 V) as compared to others. The theoretical investigations suggested that Mn-N-C catalyst possessed HOMO energy close to LUMO of O2, facilitating easy electron transfer from HOMO (3d of Mn) to LUMO (pi* of O2), weakening the O-O bond. Whereas, in the case of OER and HER of Fe-N-C catalyst, the results indicated optimum binding energy to remove O2 and H2 from the active site. This work provides a new approach to tuning the electronic and electrochemical features of the M-N-C catalyst, suggesting significant implications for catalyst design in energy conversion devices.

B12. Characterization and Biochemical Analysis of Bacteriophage Eastview9101

Gokul Maniventhan and Ismael Leon Southeastern Oklahoma State University

This study focuses on the bacteriophage Eastview9101, isolated from environmental samples, with an emphasis on its biochemical characteristics and chemical processes involved in infection. By purifying structural proteins, sequencing its genome, and conducting enzyme activity assays, we have elucidated key aspects of the phage's lifecycle. The analysis reveals how its structural proteins facilitate attachment to bacterial surfaces, how its enzymes mediate cell lysis, and how its genomic organization supports rapid replication. These findings provide a deeper understanding of phage-host interactions and offer insight into potential biotechnological applications such as phage therapy.

B13. Inhibitory Effect of Histone Deacetylase 8 by a Hydroxamic Acid Compound

<u>Evann Walker</u> and Sean Kim Northeastern State University

Histone deacetylase 8 regulates gene expression by deacetylating histones, altering chromatin structure and transcriptional activity. HDAC8 inhibitors look promising for treating cancer. Existing inhibitors lack selectivity, leading to negative effects. Developing selective HDAC8 inhibitors enhances therapeutic efficacy and minimizes adverse effects. SAHA (suberoylanilide hydroxamic acid) negates challenges, improving specificity, bioavailability, and potency, while overcoming the limitations of poor pharmacokinetics and broad HDAC inhibition. Autodock showed the compound's ability to bind strongly to HDAC's active-site, with a ΔG of -6.1 kcal/mol. Software identified two hydrogen bonds with Gly151 and Tyr306, along with a π -stacking interaction with Phe207. The compound was synthesized via a two-step method and purified using silica gel, with its purity confirmed through TLC, IR, and NMR analysis. Evaluating its effects on HDAC8, we expressed and attempted to purify HDAC8 using E. coli.

B14. Expanding the Pulay SQM Method to Modern Split Valence Basis Sets

John R. McLaughlin, Juhyeon Moon, and William B. Collier *Oral Roberts University*

The Scaled Quantum Mechanical method of Pulay is used for scaling over-estimated computed vibrational frequencies. Here it is expanded to use more modern basis sets, to see what the ultimate limit of the method may be. The popular double and triple valence sets DZV and TZV along with other basis sets are used in conjunction with the B3_LYP density functional to predict the fundamental vibrational frequencies of key organic molecules. These are least squared fitted to the experimental frequencies via the appropriate 12 Pulay scale factors. The predictive ability of the TZV basis set used in conjunction with Pulay scaling is very promising with average results near 10 cm-1 RMSD. The results and usability of this density functional with these basis sets will be examined and presented.

B15. Synthesis of Histone Deacetylase (HDAC) Inhibitor Analogs Towards Gold Nanorod Surface Coatings

<u>Charli Woessner</u>, Nathan Green, and Sean Kim *Northeastern State University*

Recent research on nanoparticles and their optical properties has led to the incorporation of nanoparticles like gold nanorods (GNRs) into various studies. In fields such as cancer therapy, techniques like photothermal therapy (PPT) are being explored for targeted drug delivery. PPT utilizes a nanoparticle's ability to convert light into heat, inducing hyperthermia to destroy cancer cells. The surface chemistry of GNRs allows attachment of molecules like folic acid, which targets folic acid receptors on cancer cells, and thiolated drug conjugates. This not only aids in hyperthermia-mediated cell destruction but also enhances drug concentration around tumors. Recent efforts have focused on synthesizing tumor-targeting and chemotherapeutic agents for GNRs using a copper-catalyzed azide–alkyne cycloaddition (CuAAC or "click") reaction. This method links azide-functionalized GNRs with alkynyl derivatives of bioactive molecules, such as

a derivative of the HDAC inhibitor vorinostat. The project aims to create bifunctionalized GNRs for targeted drug delivery and thermal therapy.

B17. Biobased Polyesters Derived from 1,4-Butanediol and a Variety of Aliphatic Diacids

<u>Vinash Chaudhari</u>, Pranabesh Sahu, and Ram K. Gupta *Pittsburg State University*\

Biobased polyesters were synthesized from 1,4-butanediol and a series of aliphatic dicarboxylic acids, namely succinic acid, adipic acid, and sebacic acid via melt polycondensation. The resulting polymers poly(butylene succinate) (PPeS), poly(butylene adipate) (PPeA), and poly(butylene sebacate) (PPeSe) were characterized with intrinsic viscosity, nuclear magnetic resonance (NMR), differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), dynamic mechanical analysis(DMA) and tensile testing. All the polymers had weight-average molecular weight over 50,000 g/mol and melting temperature (Tm) of 50-116°C, (PPeA) has low melting temperature due to semicrystalline structure and crystalize rapidly. The "even-even" effect exists as it increases tensile strength of (PPeA). All the polymers exhibit good thermal stability, mechanical properties and tensile properties compared to polyethylene. These biobased and potentially biodegradable polyester appears to be promising for practical application like packaging, biomedical materials, and environmentally friendly plastics.

B18. Performance of a DFT cluster-continuum model for predicting redox potentials of oxyanions in aqueous solution

<u>Aneeq Ahmed</u>, Cora Brown, and Gordon H. Purser *University of Tulsa*

Predicting redox potentials for difficult-to-synthesize compounds is a challenge that can be addressed by computational models. A DFT cluster-continuum model was evaluated for accuracy and cost across different computational methods, basis sets, and solvent models. Calculations on 11 oxyanions provided free energies of 43 electron transfer reactions, which were compared to experimental data. DFT performed similarly to MP2 in the gas phase, with median absolute errors (MAE) of 68.4 kJ/mol and 61.1 kJ/mol, though MP2 was not further explored. Adding diffuse functions to the basis set improved gas-phase MAE by 28%. Initially, DFT in cluster-continuum solvent performed worse than implicit solvent but better than gas-phase, but an empirical correction based on ion volume reduced errors by 65%, yielding an MAE of 30.6 kJ/mol. Converting free energies to redox potentials produced an MAE of 0.122V. The most efficient model was the volume-corrected DFT cluster-continuum model with diffuse functions.

B19. Advanced Bio-Based Polyurethane Coatings: Optimizing Strength and Hydrophobic Properties

<u>Kinal Chaudhari</u>, Mayankkumar L. Chaudhary, Rutu Patel, and Ram K. Gupta *Pittsburg State University*

Developing sustainable and high-performance coatings is crucial for replacing petroleum-based materials with eco-friendly alternatives. This study focuses on synthesizing bio-based polyurethane (PU) coatings using soybean oil polyol (SOP), glycerol (GLY) as a crosslinker, and methylene diphenyl diisocyanate (MDI). The research was conducted in two phases: first, optimizing the glycerol content to improve mechanical properties, and second, introducing hexamethyldisilane (HMDS) to enhance hydrophobicity and chemical resistance. In the first phase, PUs was prepared with varying weight percentages (wt.%) of glycerol (0, 5, 10, 15 & 20), and mechanical testing revealed that 10 wt.% GLY provided the best mechanical strength compared to other concentrations. In the second phase, this optimized formulation was further modified by adding HMDS in different wt.% (10, 20, 30, 40 & 50). The results showed that 10 wt.% HMDS provided the best tensile strength for the PU coating. However, as the amount of HMDS increased, it also shows how it affects the material crosslinks and homogeneity in the PU coating material, leading to a decrease in tensile strength, despite 10 wt.% HMDS improving the PU coating's mechanical and chemical resistance. FT-IR analysis confirmed the formation of urethane bonds, while DSC analysis validated thermal stability. Further to check the crosslinking degree of bio-based PU coatings, the samples are characterized for gel content and degree of swelling. These findings suggest that bio-based PU coatings with optimized glycerol and HMDS content can serve as a eco-friendly alternative for coatings.

B20. Evolution of Carbonaceous Aerosol from the Thermal Degradation of Plastics through Atmospheric Oxidation: From Filter-Deposited to Airborne Particles

Micah R. Miles, Katrina Betz, and Elijah J. Schnitzler Oklahoma State University Department of Chemistry

Bulk plastic samples are a known environmental pollutant and often produce secondary products throughout their lifetimes. Heated plastic samples produce nanoplastic aerosols, small particles of plastic with mobility diameters in the nanometer range that are suspended in Earth's atmosphere. Throughout their atmospheric residence time, on the order of two weeks for samples in the troposphere, the particles are subject to aging. This study focuses on aging due to ozone exposure as a function of absorbance of nanoplastic samples over time. Laboratory samples were produced by incineration of 3D-printing filament in a tube furnace or heating and extrusion through a 3D-printing nozzle. Aging was induced by the introduction of ozone, produced using a mercury bulb ozone generator. Absorbance and scattering of samples were tracked by visible spectroscopy and photoacoustic extinctiometry. Initial results show that absorption decreases significantly for deposited samples and nanoplastic aerosols during their residence time in the atmosphere.

B21. Fe(OTf)3 or Blue Light Activated Diazo-Thioglycoside Donors for Glycosylations Umesh Chaudhary, Adrienne Daróczi

The University of Oklahoma

Traditional methods for thioglycoside activation depend on expensive and toxic platinum-group metals. We present a catalytic glycosylation strategy utilizing diazo-thioglycoside donors, activated by earth-abundant iron or blue light without a photosensitizer. This approach exhibits orthogonal reactivity compared to conventional thioglycosides and alkyne-based donors, enabling one-pot glycan synthesis. The Thorpe-Ingold-like effect facilitates carbene proximity to sulfur, enhancing activation efficiency. This methodology supports various protecting groups and nucleophiles and applies to glycosyl donors such as glucose, mannose, galactose, rhamnose, xylose, lactose, 2-deoxyamino glucose, ribose, and arabinose. Additionally, it is effective for synthesizing challenging 1,2-cis furanosides, performing late-stage modifications on biomolecules like cholesterol and simvastatin at a gram scale, and enabling iterative hexasaccharide assembly. This sustainable strategy broadens the scope of glycosylation chemistry with practical and scalable applications.

B22. Optimization of reaction conditions for nucleophilic addition to 6-bromo-1,1-dichloronaphthalen-2-one

<u>Audrey A. Iskandar</u>, Steven G. Stagg, Angus A. Lamar *The University of Tulsa*

Arenols and heteroarenols are prevalent in nature and are used as building blocks in the production of FDA-approved pharmaceuticals, veterinary medicines, agricultural chemicals, and advanced materials. The predictable functionalization of an aromatic framework is a cornerstone of chemical synthesis, and significant effort has been devoted in the past century toward the development of new organic reactions to install molecular complexity to aromatic cores. Despite the intense synthetic focus, access to certain substitution patterns of polysubstituted aromatics can be restricted by intrinsic substituent effects. Specifically, an electron-donating group activates an arene toward installation of a substituent ortho or para to the original substituent via electrophilic aromatic substitution. Our recent efforts to develop a reaction to produce (hetero)arenols with rare substitution patterns will be presented.

B23. Domino Synthesis of 1,2,3,5-Tetrasubstituted 1H-Indoles

<u>Siddhartha Maji</u>, Kwabena Fobi, Ebenezer Ametsetor and Richard A. Bunce *Oklahoma State University*

A new [3+2] approach to 1,2,3,5-tetrasubstituted 1H-indoles has been developed and optimized. The method begins with the preparation of the imine from a primary benzylamine and a benzaldehyde derivative. Treatment of this imine with the K2CO3 derived anion from a methyl 2-(2-fluorophenyl)acetate substituted at C5 by an electron-withdrawing substituent yields an

adduct that cyclizes by an SNAr reaction to give the indoline. Air oxidation of the indoline then aromatizes the structure. Non-aromatic primary amines were also evaluated as reacting partners, but these gave much lower overall yields of 1H-indoles. Several sets of reactants have been evaluated and the results will be presented with a discussion of factors important to the process. All the synthesized indole derivatives (1-13) were docked to the liver X receptor alpha (PDB ID: 3IPU) receptor and compares with the LXR-623 as the standard molecule using AutoDock 4.2v tools. Compound 13 was found to be most potent.

B24. Selective N-alkylation of 1,2,4-triazoles and imidazoles

McKenzie L. Menefee, Jeanne L. Bolliger Oklahoma State University

Imidazoles and 1,2,4-triazoles are among the privileged structures which are part of many active pharmaceutical ingredients and agrochemicals. Approved drugs containing the 1,2,4-triazole unit include the antifungal agent fluconazole and the chemotherapeutic letrozole. Imidazole units are found in the antifungal drug miconazole, fexinidazole (used to treat sleeping sickness), and the agrichemical fungicide prochloraz. In this presentation we will show the selective N-alkylation of imidazoles and 1,2,4-triazoles in the presence of other nucleophilic atoms. This reaction proceeds with excellent yields and is tolerant to the presence of water and air

B25. Cross-electrophile coupling mediated by nucleophilic cobalt photocatalysis

Aishwarya Satish Nayar Oklahoma State University

Carbon radical precursors are significant in C-C bond forming reactions and have gained attention in the field of organic synthesis; however, accessibility is still underdeveloped. Nucleophilic cobalt photocatalysis can be employed in carbon centered radical formation to enable umpolung reactivity of unconventional electrophilic precursors. Square planar cobalt complexes, such as cobaloximes and Vitamin B12, are known to achieve nucleophilicity in the Co-(I) oxidation state and undergo SN2 type reaction with various electrophiles. The resulting Co-C bond can undergo facile photolysis to afford radicals that are useful for several transformations. This work employs Co(salen)2 as a nucleophilic photocatalyst for the cross coupling of Michael acceptors and Eschenmoser's salt. The reaction proceeds through a α -aminoalkyl radical intermediate formed from the reaction of Co-(I) and Eschenmoser's salt, followed by Giese-type addition with the Michael acceptor to give the cross coupled product. Preliminary results and reaction optimization studies will be presented.

B26. Benzo[d]oxazoles from Anilides by N-Deprotonation-O-SNAr Cyclization

<u>Nash E. Nevels</u>, Luke Subera, and Richard A. Bunce *Oklahoma State University*

A synthesis of benzo[d]oxazoles by an N-deprotonation—O-SNAr cyclization sequence from anilide precursors is reported. Anilides derived from 2-fluoroanilines, activated toward SNAr ring closure by C5 electron-withdrawing groups, were prepared and subjected to deprotonation—cyclization using 2 equiv. of K2CO3 in anhydrous DMF. Following deprotonation at nitrogen, the delocalized anion cyclized from the amide oxygen to give high yields of benzo[d]oxazoles. The temperature required for the cyclization of benzanilides correlated with the potency of the C5 activating group on the SNAr acceptor ring with nitro (most potent) reacting at 90 C (1 h), cyano reacting at 115 C (1 h), methoxycarbonyl reacting at 120 C (2 h), and trifluoromethyl (least potent) reacting at 130 C (3 h). Acetanilides were more difficult to cyclize but generally required 4–6 h at these same temperatures for completion.

B27. Mechanistic study in new synthetic methods of N-alkenyl 1,2,4-triazolones and 1,3-imidazolones

<u>Abigail C. Norris</u>, Jeanne L. Bolliger *Oklahoma State University*

The 1,2,4-triazolone unit has been found in several biologically active compounds that have been used to treat liver-fat buildup and hypertension. Although there are a few patents, we have only found a couple research articles for the preparation of these scaffolds involving toxic catalysts. We have discovered a new, safer synthetic route for the preparation of differently substituted 1,2,4-triazolones as well as 1,3-imidazolones. We can successfully obtain N-alkenyl substituted triazolones and imidazolones via an oxidative cyclization followed by a rearrangement.

B28. Bromination of Indazole and Pyrazole Derivatives via Organocatalytic Activation of N-Bromosuccinimide

Muhammad Qasid, Angus A. Lamar *The University of Tulsa*

Halogenation of aromatic and heteroaromatic compounds is one of the most widely employed reactions in medicinal chemistry to synthesize biologically active compounds. In addition, halogenation is viewed as an effective method to produce intermediates for the installation of additional functionality through cross-coupling reactions. Our research group has previously shown that visible-light photoredox catalysis (VLPC) is a useful approach to aid in the non-acidic, electrophilic halogenation of aromatic and heteroaromatic compounds. In a recent investigation, we have observed the activation of N-bromosuccinimide (NBS) by organic dye catalysts in the absence of light. We have identified an organocatalyst and optimized the reaction conditions for bromination of a representative indazole in the absence of light. Our progress towards the investigation of the substrate scope (indazole and pyrazole) for the organocatalyzed bromination reaction is presented.

B29. Alkoxy Substituent Variation of Ethyl 4-((4-methoxybenzyl)thio)-3-(4H-1,2,4-triazol-4-yl)benzoic Acid

<u>Kaitlyn M. O'Brien</u>, Jeanne L. Bolliger *Oklahoma State University*

It is known that many azoles, polyenes, and allylamines have antifungal properties. The purpose of this research is to chemically modify one of our lead compounds which contains an azole, more specifically a triazole unit, in hopes of forming a more effective antifungal agent to target the opportunistic pathogenic yeast, Candida Albicans. Since our lead compound had an ester functionality, we decided to explore the effect of the alkoxy substituents on the antifungal activity. For this we prepared a common carboxylic acid precursor which then was converted in two steps to a range of ester analogues.

B30. Biomolecule Conjugation to Dye-Doped Silica Nanoparticles

Brandi P Woods, Nathan S Green Northeastern State University

Silica nanoparticles (SiNP) are versatile, bioinert, and highly customizable nanospheres that have been pursued for cutting edge applications in the medical and materials fields. Here we report on recent progress of surface functionalized dye-doped SiNPs with potential uses such as energy transfer complexes, water purification, fluorescent signaling, and self-assembly. The SiNPs are grown in shells which allow for careful control over size and molecular doping of the silica interior. The shell growth provides a silanol surface where free hydroxyl groups can be functionalized with a range of small organic functional groups. These surface functionalities allow for further attachment to other nanoparticles and biomolecules like DNA and proteins. The present study focuses on rhodamine B dye-doped silica nanoparticles with amine coatings for protein attachment. The goal of this project is to produce highly customizable nano-engineered SiNP that can be easily incorporated into a number of medical and material applications.

B31. Vitamin B₁₂ Electrochemistry Using Electrodes

<u>Paige M Robertson</u>, Subrata Pal *Oklahoma State University*

Vitamin B12, also referred to as cobalamin, is renowned for its superlative nucleophilic properties, which can be leveraged in SN2-type reactions with electrophiles, like acetic anhydride. The intermediate, Co(III)-carbonyl, contains a weak Co(III)-C bond which can be cleaved homolytically upon irradiating visible light to generate an acyl radical. While others are using external reducing agents, such as Zn or Mn metal, to access the nucleophilic Co(I) oxidation state, we are using an electrochemical approach. In this work, our progress towards developing a photo-electrochemical Vitamin B12-catalyzed Giese reaction will be presented. Our efforts towards optimizing both the electrochemical cell and reaction parameters, including utilizing different counter electrodes like Zn, Mg, glassy carbon, etc., will be presented.

B32. Two-Step Synthesis of 1,2,4-Trisubstituted Naphthalene Analogs

Steven G. Stagg, Audrey A. Iskandar, Angus A. Lamar *The University of Tulsa*

Electrophilic aromatic substitution, cross-coupling reactions, and direct metalation reactions are three of the most common reactions in medicinal chemistry used to modify aromatic scaffolds. These three reaction classes each provide regioselectivity which can be advantageous or limiting depending on the desired structure. Our lab is interested in developing new methods to produce aromatic scaffolds with rare substitution patterns that are difficult to produce by other means. Our recent progress toward the development and optimization of a two-step, one-pot reaction to install functionality on an aromatic core is presented.

B33. Synthesis of 4-(tert-butyl) Pyridine from DHP and 4-Cyanopyridine Utilizing Photo Mediated Redox Processes

<u>Kayman B. Ross</u>, Viraj K. Arachchige, and Spencer P. Pitre *Oklahoma State University*

The generation of tertiary radicals via photo-mediated redox processes represents a significant advancement in the introduction of sp³-hybridized carbons, which are crucial in pharmaceutical research. Traditional methods for generating tertiary alkyl radicals often rely on an exogenous photocatalyst, which are typically precious-metal complexes, and current photocatalyst-free approaches often involve hazardous reagents and complex procedures, posing safety and reproducibility challenges. Inspired by our lab's prior work, we present a safer and more efficient photocatalyst-free approach by utilizing 4-tert-alkyl-1,4-dihydropyridine (DHP) derivatives as tertiary radical precursors under visible light irradiation for sp3-sp2 C-C coupling reactions. Our progress in the optimization of key variables, including solvent concentration, light intensity, and reaction time, which were systematically explored to enhance yield and selectivity will be discussed. This research contributes to the development of greener and more sustainable synthetic methodologies in organic chemistry, addressing prior limitations in safety and reaction control.

B34. Study of iodine distribution and concentrations in western Oklahoma brine waters and recycling of used chloroform

Amanda Lane, Alaina Pierce, Jason R. Wickham, Averie Larson, Josena Frame, Kathryn Baugh, and David Edlin Northwestern Oklahoma State University

In the late 1970's, it was discovered that the brine waters of NW OK contain significant amounts of Iodine (above 60 ppm). However, the exact amounts and distributions of Iodine throughout this region were unknown. Currently, the majority of the world's supply of Iodine comes from mining Iodate minerals in Chile (\approx 65%), brine water aquifers in NW Oklahoma (\approx 5%) and Japan (\approx 25%), and seaweed extraction. With the growing need for Iodine compounds in various fields the demand for Iodine is higher than ever. Thus, Iofina and NWOSU created a partnership to quantify the Iodine concentrations and distribution throughout the brine aquifer, as well as, determine the longevity of these iodine concentrations. So far, this study has led to the discovery of new sites

within the aquifer that may be of commercial interest and has taken an in-depth look at several possible new plant sites, which has led to the construction of six new plants. Fluctuations in iodine concentrations of up to 100 ppm have been observed throughout this study which is a much larger fluctuation than the expected 10 ppm. We are currently investigating rather these fluctuations are due to the changed from vertical to horizontal wells as a function of the inhomogeneity within the brine aquifer. Iofina currently uses chloroform during routing testing procedures during plant operations. In order to reduce the financial and environmental impact of this chloroform waste we have generated a distillation process to recycle this chloroform with up to a 93% recovery.

B35. Halogen-Bonding Photocatalysis Using Carbazoles as Electron Donors

<u>Samuel J Scovitch</u>, Tarannum Tasnim, Negin Shafiei, and Spencer P. Pitre *Oklahoma State University*

Charge-transfer complexes (CTCs) form when an electron-rich donor molecule interacts with an electron-deficient acceptor molecule in solution. This interaction produces a lower-energy molecular system compared to the separate donor and acceptor, causing the complex to absorb in the visible region. As a result, visible light can excite the CTC, leading to intra-complex single-electron transfer followed by the potential generation of radical species. A common strategy for producing CTCs involves halogen bonding, in which an electron-rich donor interacts with the sigma hole of a halogen atom (Cl, Br, or I). Notably, 2,5-di-tert-butylhydroquinone has been shown to effectively catalyze radical formation through a halogen bonding interaction with fluoroalkyl iodides under visible light irradiation. Up to this point, alkyl chlorides have not been successfully utilized as radical precursors, due to their small sigma holes, prompting the need for a catalyst with stronger electron-donating capabilities. We hypothesized that a carbazole-based analog could offer this enhanced electron donation and thereby enable radical formation from alkyl chlorides. Our investigations into the structure-activity relationships of the carbazole catalyst, reaction optimization, and our progress towards the reaction scope will be discussed.

B36. Assessing Forever Chemical Contamination in Northeastern Oklahoma Using LC MS/MS

<u>Baboucarr Awe</u>, Foysal Md. Hasan, Ismail Erfan, and Kenneth Roberts *The University of Tulsa*

Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants with significant ecological and human health concerns. This study focuses on assessing PFAS contamination in Northeastern Oklahoma, analyzing water, sediment, and bioaccumulation in fish and mussels using liquid chromatography-tandem mass spectrometry (LC-MS/MS). By quantifying PFAS levels and investigating their metabolic pathways in aquatic species, this research will provide critical data on how different organisms accumulate and process various PFAS compounds. Sampling from multiple river sites will allow for a comprehensive analysis of spatial contamination trends, identifying potential hotspots. Given the limited studies on PFAS contamination in this region, the findings will contribute to improved risk assessment, regulatory action, and remediation strategies. This research aims to enhance the understanding of PFAS

distribution in aquatic ecosystems, ultimately supporting efforts to protect water quality, public health, and environmental sustainability.

B37. Generation of Light-Absorbing Carbonaceous Aerosol from Thermal Degradation of Plastics and Whitening through Atmospheric Irradiation

Asma Soofi, Elijah Schnitzler Oklahoma State University

Carbonaceous particles suspended in air can be carried great distances by wind currents and have significant effects on cloud formation, climatic patterns, and human health. Plastic incineration is a growing source of carbonaceous aerosol. In this study, we investigate how exposure to sunlight affects the light absorption of carbonaceous aerosol from the thermal degradation of plastics. Aerosol was generated by heating red, colorless, and blue polyethylene terephthalate glycol (PETG) and acrylonitrile butadiene styrene (ABS) filaments in a tube furnace. A range of furnace temperatures was explored, from 300 to 500oC, for all filaments. The resulting nanoparticles were collected on quartz fiber filters. Filter-deposited nanoparticles were exposed to light from a Xe lamp in a solar simulator for four days. The light absorption of the samples at visible wavelengths was monitored in 24-hour intervals. These results help us constrain the lifetime and climate impacts of this class of carbonaceous aerosol.

B38. Temporal analysis of Kiamichi river water quality using mollusk bioindicators

Erfan Smiley and Dr. Kenneth Roberts *The University of Tulsa*

This study investigates the temporal variations in water quality of the Kiamichi River using mollusk bioindicators. Mollusks, as sensitive aquatic organisms, provide valuable insight into the river's ecological health by bioaccumulating contaminants over time. Water samples and mollusk specimens were collected seasonally from multiple sites along the river, and their heavy metal concentrations, stable isotope ratios, and physiological responses were analyzed. Additionally, physicochemical parameters such as pH, dissolved oxygen, and nutrient levels were monitored to correlate environmental changes with mollusk bioindicators. The results revealed seasonal fluctuations in water quality, with increased pollutant accumulation during periods of high runoff and anthropogenic activity. Statistical analyses confirmed significant correlations between mollusk bioaccumulation trends and water quality parameters. These findings highlight the potential of mollusks as reliable bioindicators for long-term water quality assessment, aiding in conservation efforts and informed management of freshwater resources in the Kiamichi River basin.

B39. DOM in Oklahoma Waters

<u>Colter I Bufford</u>, Shawna York Southern Nazarene University

Dissolved organic matter (DOM) is a heterogeneous mixture of organic compounds that take place in natural waters across the world. DOM and its major subset colored dissolved organic matter (CDOM) affect important environmental processes like the carbon cycle that influence climate change. We have done a systematic analysis using UV-VIS spectroscopy, FT-IR spectroscopy, and proton NMR to help analyze the structures and functional groups of compounds in lake water. Water samples were first characterized without pretreatment by measuring conductivity, pH, and turbidity to help compare water from different sources. Lake sample waters all had statistically the same pH but varying conductivity and turbidity. Our FT-IR results showed significant similarities with chlorophyll with amounts varying by water source. Our 1H-NMR indicated the existence of carboxyls and aliphatics within the waters. Finally, the UV-Vis spectra showed low absorbance throughout the visible spectrum but a high absorbance in the UV-C region.

B40. Comparative Analysis of Green Synthesized Silver Nanoparticles from *Citrus limon*, *Citrus reticulata*, and *Citrus sinensis* Fruit Peel Extracts

<u>Isabel Ray</u>, Gershom Smith, Stormy Haynes, and Deshani Fernando *Mid-America Christian University*

The environmental impact of discarded citrus peels is a growing concern. Given their rich citric and ascorbic acid content, citrus fruits are increasingly explored for silver nanoparticle (AgNP) synthesis. While studies confirm AgNP synthesis using aqueous citrus peel extracts, a comparative assessment of *Citrus limon*, *Citrus reticulata*, and *Citrus sinensis* extracts remains unexplored. This study synthesized AgNPs from these extracts and characterized them via UV–vis spectrometry, FTIR, and TEM. The one-factor-at-a-time optimization technique was used to assess the effect of temperature, volume ratio, and reaction time. All three extracts exhibited a maximum production of AgNPs at 50 °C while treating 1 mL of peel extract with 9 mL of 1 mM silver nitrate. The color change, from pale yellow to brown, and UV-vis analysis confirmed AgNP biosynthesis. *Citrus reticulata* yielded the highest AgNP concentration with a smaller particle size. FTIR analysis identified functional groups responsible for capping and stabilization.

B41. Influence of Crosslinkers on the Mechanical and Thermal Characteristics of Bio-Based Polyurethane Adhesives

<u>Jaymin Joshi</u>, Mayankkumar L. Chaudhary, Rutu Patel, and Ram K. Gupta *Pittsburg State University*

The development of sustainable adhesives with enhanced mechanical, thermal, and chemical properties is essential for industrial applications. This study focuses on synthesizing polyurethane adhesives using soybean oil polyol (SOP) and methylene diphenyl diisocyanate (MDI), incorporating dimethyl terephthalate (DMT)-derived crosslinkers, DEA and DPA, to enhance mechanical performance. The influence of crosslinker type and concentration on adhesive

properties was investigated by preparing adhesives with varying crosslinker weight percentages (wt.%) (5, 10, 15, and 20 for DEA and 5, 10, 15, 20 and 25 for DPA) and curing them at room temperature (RT). Fourier Transform Infrared Spectroscopy (FTIR) confirmed urethane linkage formation, while tensile strength testing on oak wood showed an increase in strength with crosslinker concentration up to an optimal level. The highest tensile strength for DEA-based adhesives was 6.77 MPa at 15 wt.%, decreasing to 4.1 MPa at 20 wt.%. Similarly, DPA-based adhesives exhibited peak tensile strength of 6.86 MPa at 20 wt.%, reducing to 4.26 MPa at 25 wt.%. The improved mechanical performance was attributed to noncovalent interactions between PU molecules and the substrate surface. Differential Scanning Calorimetry (DSC) analysis assessed thermal stability, while gel content and swelling degree confirmed crosslinking. These findings contribute to developing high-performance polyurethane adhesives for diverse applications.

B42. Bio-Based Thermosets: Influence of Various Diols and Diisocyanates

Mayankkumar L. Chaudhary, Rutu Patel, and Ram K. Gupta *Pittsburg State University*

The multipurpose polymers known as polyurethanes (PUs) have many different uses. Traditional PUs, on the other hand, frequently use polyols derived from petroleum, which are very harmful to both humans and the environment. Sustainable alternatives, such as bio-based polyols, have arisen to deal with these problems; in particular, polyols derived from vegetable oil (VO) have been the subject of much research due to their ability to lessen the need for fossil fuels. Mechanical strength is a common issue with bio-based PUs, despite their environmental benefits. The objective of this research is to improve the mechanical properties of bio-based PUs by using aliphatic (1,3-propanediol, or PR) and aromatic (1,5-pentanediol, or PN) and hydroquinone, or HQ, diols as cross-linkers. The impact of several aromatic and aliphatic diisocyanates on thermosetting PU production is now being studied. The PU films' mechanical strength and rigidity are aimed to be increased by manipulating these cross-linkers and diisocyanates. The tensile strength of samples containing methylene diphenyl diisocyanate (MDI) increased significantly with the addition of HQ (10 wt.%), reaching around 40 MPa, compared to 6 MPa in the control samples. The PU film with the most hexamethylene diisocyanate (HDI) had the greatest tensile strength of 9 MPa, which was achieved by a PR film with 15 wt.% of HDI. Furthermore, films containing HDI demonstrated better elongation in comparison to films containing MDI. Additional tests to evaluate the PU films' cross-linking and stiffness included thermal investigations, gel content analysis, and swelling degree.

B44. Core-Shell Silica Nanoparticle Synthesis and Surface Functionalization

<u>Brenna K.Y. Maynard</u> and Nathan S. Green *Northeastern State University*

Silica nanoparticles (SiNP) have been readily synthesized since the 1960s and have shown remarkable potential in their customization. The preparation of silica nanoparticles starting with core growth and followed by outer shell regrowth allows their size to be tailored for specialized applications. The high surface area-to-volume ratio and surface modifiability of silica

nanoparticles further add to their capacity for functionalization. Here we report on recent progress towards developing dye-doped silica nanoparticles through the shell regrowth process. The silica shell regrown over the dye-doped layer acts as a shield, protecting the functional properties of the dye from being diminished by leaching and photobleaching, as well as providing a surface to functionalize with reactive additives. Combining these fluorescent dye-doped silica nanoparticles with additional nanomaterials, such as gold nanorods, allows for a novel model to transfer energy across the nanoscale. Coating the SiNP surface with ssDNA enables these model systems to self-assemble with high fidelity. These self-assembled hetero-nanoparticle assemblies have potential applications in solar capture, signaling, and fluorescent imaging.

B45. Electrochemical Measurement of Freeze-Thaw Cycle Impact on Sarcoplasmic Oxidation in Beef

<u>Silan Bhandari</u>, Sachinthani A. Devage, Rishav Kumar, Dr. Ranjith Ramanathan, and Dr. Sadagopan Krishnan *Oklahoma State University*

Repeated freezing and thawing (F-T) of meat products occurs in-home kitchens, markets, and transportation which reduces quality of meat due to wider fluctuations in temperature. This study introduces the first electrochemical analysis of oxidation in beef longissimus lumborum (LL) muscle sarcoplasm during repeated F-T cycles. The approach is a low-cost, highly sensitive, and selective alternative to traditional techniques (e.g., Raman, NMR, FTIR), effectively detecting protein oxidation. In this study, increased current responses measured electrochemically correlated strongly with elevated metmyoglobin content. This study emphasizes F-T cycles decrease meat quality when exceeds above the third cycle. This research introduces a portable, cost-effective electrochemical tool for point-of-need monitoring of meat oxidation under various practical, experimental and environmental conditions.

B46. Non-Enzymatic Glucose Detection using Spray Painted Electrodes from 3D Printed Masks

<u>Ashlyn Stephenson</u> and Gabriel LeBlanc *The University of Tulsa*

This study focuses on the development of glucose sensing electrodes fabricated using 3D-printed masks on glass microscope slides. The 3D mask and microscope slides ensure replicability of the electrodes, while maintaining the ability to generate unique designs at low cost. Nickel spray paint is used to create the electrode on the glass surface, followed by electrodeposition of copper on the working electrode to enhance its sensitivity to glucose. This method provides an accessible and efficient approach for creating low-cost electrochemical sensors that can be applied to glucose monitoring systems while demonstrating the potential of this general method for analysis of a wide range of analytical targets.

B47. Sensitive and selective label-free capacitance sensor for infectious biomolecule

detection

<u>Sathya Samaraweera</u>, Joshua D. Ramsey, and Sadagopan Krishnan *Oklahoma State University*

Infectious biomolecule detection is critical in diagnosing diseases, as the process needs to be more sensitive and selective. Common methods like RT-PCR (105 copies/mL) and antibody-based methods (1011 copies/mL) are selective; however, they possess limitations such as special laboratory skills, longer assay times, and complex tagging or labeling methods. Electrochemical Impedance Spectroscopy (EIS) is an electrochemical technique that facilitates label-free detection of biomolecules with high sensitivity and selectivity. In this study, we introduce a pyrenyl-nanocarbon-modified electrode to detect femtomolar-level ~105 copies/mL target SARS-CoV-2 RNA by measuring the interfacial capacitance changes. This approach will eliminate the use of chemical and enzymatic tags used in common immunoassays, enhancing the rapid and robust detection of target biomolecules quantitatively. This sensor can be applicable on different platforms, potentially in clinical studies to diagnose various infectious biomolecules at their early stages.

B48. Spatiotemporal Assessment of Trace Metal Contamination in the Kiamichi River, Oklahoma

Md Foysal Hasan, Lauren Haygood, Baboucarr Awe, Erfan Smiley, and Kenneth Roberts

The University of Tulsa

The Kiamichi River plays a crucial role in supporting Oklahoma's freshwater ecosystems. Recent climatic shifts since the 1990s, worsened by hydrologic drought (USGS streamflow index), coupled with Oklahoma City's proposed water extraction, raise concerns over ecological impact. This study evaluates the impacts of natural drought and anthropogenic activity on the river's water geochemistry, including heavy metals. At least 10 sites were selected based on development activity for in-situ measurements and lab analysis. Water in-situ measurements from summers 2023 and 2024 showed slightly acidic conditions. Trace metal analysis using inductively coupled plasma mass spectrometry (following EPA guidelines) revealed elevated concentrations of heavy metals, including zinc, chromium, copper, and nickel, in the river's downstream sites. Ongoing investigations aim to assess trace metals and source apportionment of these metals, with the goal of informing policy bodies to make proper management strategies to safeguard the ecological balance of this vital river basin.

B49. The Chemistry of Artificial Sweeteners

<u>Arastu Manral</u> and <u>Andrew Wang</u> Oklahoma School of Science and Mathematics

Diet Sodas, chewing gums, and other popular foods typically contain artificial sweeteners. These artificial sweeteners are used to enhance sweetness while reducing caloric intake. Chemically, they vary in structure. Some are peptides, like aspartame. Others may be sulfonamides, like saccharin. Their sweetness intensity often surpasses sucrose by hundreds of times, enabling minimal usage in food products. However, these artificial sweeteners have potential hazards that could lead to fatal situations. Research on their safety and health effects, including potential diseases like cancer or heart attacks, continues to evolve. Understanding their chemistry is essential for optimizing their usage in food science. In this project, we will investigate the chemistry of artificial sweeteners such as aspartame and saccharin, then discuss future research that could be conducted, with a special focus on their effects in the food industry.

B50. Meat Science: Determining the species-specific heme protein redox behavior using an electrochemical approach

<u>Sachinthani U.K Ayabadda Devage</u>, Silan Bhandari, Minha Arankuny, Ranjith Ramanathan, and Sadagopan Krishnan *Oklahoma State University*

The sarcoplasmic heme protein, myoglobin, mainly determines meat color. There are slight differences in the structure of myoglobin of each species. The difference in amino acid sequence determines the net charge of protein and its affinity to oxygen binding. With the aid of biochemical insights, electrochemical measurements were performed using square-wave voltammetry (SWV) and high-purity graphite (HPG) electrodes to identify the species-specific redox behavior of heme proteins of beef, chicken and pork. Beef showed a distinct high intense reduction peak at -0.27 V compared to both pork and chicken species. The first oxidation peak at 0.36 ± 0.01 V obtained in the positive potential region is more prominent and intense in chicken than the other two species, which correlates with the elevated metmyoglobin percentages leading to high oxidative processes. This work shows the species-specific redox characteristics and highlights the potential of biochemical and electrochemical approaches to assess meat quality.

B51. Electrodeposition of Metal Oxides for Use in Perovskite-Based Solar Cells

McCaleb L Doyle, Ethan Falconetti, Julian Talmon, and Gabriel LeBlanc *University of Tulsa*

Today, almost all commercially available solar cells are made using very high purity silicon, purified with methods that use large amounts of energy and money. This research aims to create low-cost and scalable solar cells using electrodeposition of both perovskite precursor and metal oxide electron transport layers. Electrodeposition is favored for its cost efficiency, scalability, and precise control it enables over chemical-based depositions. In this research, the metal oxides of focus were tin and niobium oxide. The metal oxides were electrodeposited using chronoamperometry with a three-electrode setup on a potentiostat. Their consistency and thickness were evaluated using contact profilometry, atomic force microscopy (AFM), x-ray diffraction (XRD), and spectrophotometry. The ability to deposit metal oxide on flexible substrate with a low-cost and low-temperature method such as the electrodepositions used opens the door to lower-cost manufacturing methods as well as lighter and more flexible solar cells.

B52. Bio-Based Adhesives: The Role of Diamine and Triamine Cross-Linkers in Soybean Oil-Derived Non-Isocyanate Polyurethane

Sauravkumar Patel, Chandan Bodhak, and Ram K. Gupta *Pittsburg State University*

Polyurethanes (PUs) are essential in the polymer industry due to their unique mechanical and chemical properties in foams, paints, coatings, elastomers, and adhesives. Bio-based sources, such as soybean oil (SBO), offer a sustainable alternative to petroleum-based materials. This study explores non-isocyanate PUs (NIPUs) for their sustainability and lower toxicity. SBO was converted into epoxidized soybean oil (ESBO), then into CSBO using a Parr autoclave reactor with tetrabutylammonium bromide (TBAB). CSBO was characterized via FT-IR, %EOC content, viscosity, GPC, and ¹H NMR. NIPUs were synthesized using solvent- and catalyst-free methods with diamines (Isophorone diamine, Meta-xylylenediamine) or triamine (Tris(2-aminoethyl)amine). FT-IR tracked reaction progress, while TGA and DSC assessed thermal properties. Adhesion tests on wood (oak) and metal (stainless steel) showed strong bonding via noncovalent interactions. Wood adhesive failure in TAA-based NIPU indicated bonding failure. The polymer's crosslinking was confirmed by adhesive gelling data.

B53. Transistor Technology: Fast, Present & Future

<u>Bishal Lamichhane</u> and Delwar Hossain Oklahoma School of Science and Mathematics

Transistors are an essential component of electronic devices, enabling advances in communications, computing, healthcare, military systems, transportation, clean energy, and countless other applications. Transistors are the heart of one of the semiconductor chips. All transistors are interconnected and act as switches for electrical current. These gates turn on and off, allowing or preventing current from passing through. As the size of the transistors decreases, the evolution of electronic chips increases exponentially. But, Moore's law no longer applies to electronic chips and is

almost within its limit. To keep Moore's law alive, the miniaturization of transistors becomes essential. This presentation discusses a brief review of the transistor's past and present and presents a future research plan.

B54. Two-stage Transesterification and Melt Polycondensation for the Synthesis and Characterization of Bio-Based Aliphatic Polyesters

<u>Rutu Patel</u>, Mayankkumar L. Chaudhary, and Ram K. Gupta *Pittsburg State University*

One of the biggest problems in modern polymer research and engineering is coming up with eco-friendly and long-lasting polymer materials. The adaptability and versatility of bio-based polyesters have made them a hot topic as possible solutions. New bio-based polyesters have emerged in recent years, fueling the expansion of the bio-based sector. This is all thanks to improvements in the methods used to prepare bio-based monomers. The diols 1,3-propanediol (13) and 1,5-pentanediol (15) and the diacids adipic acid (AD) and sebacic acid (SB), some of which may be bio-based, are the main ingredients in this study's aliphatic polyester synthesis, which employs a transesterification and melt polycondensation technique. The AD+13 polyester had the largest molecular weight out of all the polyesters, which varied from 17,198 to 42,924 g/mol. Decomposition temperatures above 300°C and melting points between 38°C and 55°C were indicative of strong stability according to thermal analysis. The mechanical performance of polyesters based on SB was lower, while AD+15 polyester exhibited the highest tensile strength (750 KPa) and elongation (360%). Tests for solubility verified that chloroform and toluene, among other solvents, were compatible with polyesters. Based on these results, the bio-based polyesters that were made in this research could be great for eco-friendly packaging and coatings.

Efforts Towards the Development of a Synthetic Pathway for Catenulobactin B and Its Analogs: A Step Forward for Novel Antibiotic Delivery Systems

<u>Theodore N Quarcoopome</u>, Arielle Whitner, and Prathibha Desman Patel *Oral Roberts University*

Catenulobactin B is a novel heterocyclic polypeptide isolated from Catenuloplanes sp. by Abe et al. in 2018. To date, its total synthesis has not been reported. Our research group is developing a synthetic route for Catenulobactin B and its analogs to facilitate biological and structural investigations. Initial efforts focus on synthesizing the first analog, Cat 1, which retains the core Catenulobactin B scaffold but is easier to synthesize. This stepwise approach involves peptide coupling, oxazoline ring formation, and saponification, followed by protection and deprotection of an ornithine group. Catenulobactin B is a siderophore that bacteria use to acquire iron from the environment. When conjugated with antibiotics, siderophores form sideromycins, which bypass the porin channels of gram-negative bacteria, enhancing antibiotic uptake. Upon completion of Catenulobactin B and its analogs, they will be used to synthesize novel sideromycins, enabling further research into their potential to improve antibiotic efficacy.

B56. Developing FeCo-NC alloy for optimizing electrocatalytic activity in water splitting and oxygen reduction

<u>Harsh Panchal</u>, Ronit Chaudhari, Kemilaben Chaudhary, and Ram K. Gupta *Pittsburg State University*

The increasing demand for sustainable energy solutions has driven extensive research into efficient and cost-effective electrocatalysts for key electrochemical reactions, including the OER, HER, and ORR. This study focuses on the development of a FeCo-NC/CNT alloy catalyst with tunable Fe/Co ratios to optimize electrocatalytic performance in these critical reactions. The FeCo-NC/CNT catalyst was synthesized using hydrothermal and pyrolysis techniques, ensuring the formation of a well-defined alloy structure with nitrogen-doped carbon support. Characterization confirmed the successful incorporation of Fe and Co into the NC/CNT framework, enhancing electrical conductivity and the density of active sites. Electrochemical evaluations revealed that the Fe0.9Co0.1-CNT composition exhibited superior catalytic activity, achieving an overpotential of 247 mV for OER and 71 mV for HER at a current density of 10 mA/cm², along with an ORR half-wave potential (E1/2) of 0.87 V vs. RHE. Notably, the OER performance of the Fe0.9Co0.1-CNT catalyst approaches that of Iridium Oxide, a benchmark noble metal catalyst, demonstrating its potential as an efficient and cost-effective alternative. The synergy between Fe and Co within the NC/CNT matrix significantly enhances reaction kinetics and electron transfer, improving catalytic efficiency. The findings indicate that the FeCo-NC/CNT alloy catalyst presents a promising pathway for replacing expensive noble metal-based electrocatalysts in fuel cells, metal-air batteries, and water-splitting systems. This study highlights the importance of tuning metal composition and structural engineering to achieve high-performance catalysts, contributing to the advancement of sustainable energy technologies.

B57. Introducing Simpler Chemistry- A New Approach

Odilia N Osakwe Tulsa Community College

Simpler Chemistry by Dr. Odilia Osakwe is an innovative thoughtfully crafted companion book designed to improve the comprehension of introductory chemistry making it more accessible and engaging for learners. This book was born out of a desire to provide clarity to the recurring questions and misconceptions that students often raise, but which are rarely addressed in traditional textbooks. The chapters in this book provide an easy-to-follow introduction to core concepts with multiple solution pathways as strategies for exploring more advanced ideas later in the course. Simpler Chemistry not only benefits students by making the subject more approachable but also supports educators by providing a reliable resource for effective teaching. This book is ideal for high school students, college freshmen, or anyone new to the field who seeks a structured and supportive guide through the foundations of chemistry. The attractive features of this book highlights will be presented.

B58. Electrodeposition of Catalytic Platinum on 3D Printed Nickel Electrodes

<u>Chetna Mandurai</u> and Gabriel LeBlanc *University of Tulsa*

Platinum is a highly effective catalyst for numerous electrochemical reactions, including water electrolysis. However, its high cost and the challenge of finding electrodes with suitable geometries for specific applications limit widespread use. To address this, our research group has developed a technique to fabricate custom electrodes by modifying 3D-printed substrates with conductive nickel paint, yielding electrodes with excellent conductivity for various electrochemical processes. Despite their versatility, these electrodes are constrained by the inherent properties of nickel. In this study, we enhanced the catalytic performance of the nickel electrodes by electrodepositing various platinum salt solutions. We optimized deposition conditions, and then evaluated the resulting platinum-modified electrodes. Their electrocatalytic efficiency was assessed through water electrolysis, demonstrating a significant reduction in the overpotential required compared to the unmodified nickel electrodes. This approach offers a cost-effective strategy for enhancing the performance of 3D-printed electrodes, making them suitable for a broad range of electrocatalytic applications.

B60. Electrodeposition of ZnO on Plastic-Based Substrates for Solar Cell Applications

<u>Maivi Nguyen</u> and Gabriel LeBlanc *University of Tulsa*

Perovskite-based solar cells have sparked enthusiasm in the research community due to the ability to employ lower cost processing methods. In these systems, the electron-hole pairs generated by the perovskite material move electrons through different layers to enhance the efficiency of the charge separation. Many of the methods currently used to generate the different layers are difficult to scale and require high temperatures. Electrodeposition, however, is considered very scalable and often requires much lower temperatures. Here we describe the formation of thin ZnO films on ITO-PET substrates at relatively low temperatures (70°C). After confirmation of the crystalline ZnO using XRD, the electrodeposition process was altered in order to increase the density of the ZnO film and minimize the light scattering effects. The electrodeposition of a more transparent and crystalline ZnO film on inexpensive ITO-PET electrodes provides the opportunity to use this electron transport material in low cost and scalable perovskite-based solar cells.

B61. Computational and Experimental Study of Amine-Based Sorbent for CO2 capture at low Pressure

<u>Aaron T. Caesar</u> and Nicholas F. Materer Oklahoma State University

The amine-based sorbent removal media for CO2 offer multiple advantages, high adsorption capacity, high adsorption rate, moisture tolerance and being easily regenerable over the traditional calcium hydroxide. Primary amines have the highest affinity for acidic CO2 but provide less regeneration because of the stronger chemical interaction. To adjust the CO2 capture sorbent to be more readily regenerated, secondary and functionalized primary amines were model as substrate. Computational simulations were used to model the interaction between CO2 molecules and methylamine. This provides insights into reaction pathways and energetics for adsorption of CO2 using amine supported with polymeric material. BET adsorption-desorption for CO2 was also used to study their uptake capacity at relative pressure.

B62. Cost-Effective Fabrication of Ag/AgCl Reference Electrodes for Electrochemical Applications

Abigail Ott and Gabriel LeBlanc University of Tulsa

In electrochemistry, applying a stable and precise reference voltage is essential for accurate experimental results. This is commonly achieved using Ag/AgCl reference electrodes. Although commercial electrodes are readily available, the ability to fabricate custom reference electrodes provides flexibility for specialized experimental setups and reduces costs. This study investigates the development of cost-effective Ag/AgCl reference electrodes by modifying 3D-printed substrates and spray-coated surfaces. We evaluated the performance of these custom electrodes, including their use as pseudo-reference electrodes and their enhancement with silver paint to create traditional Ag/AgCl electrodes. The electrodes' voltage stability was tested using standard electrolytes and benchmarked against commercial reference electrodes. Long-term stability was also assessed to ensure reliability over time. By enabling the fabrication of low-cost, custom-shaped reference electrodes, this work opens the door to wider accessibility and tailored designs in electrochemical experimentation.

B63. Colorimetric Hybridization sensor mechanism for multiple target detections

<u>Colton J. Scott</u> and Aubri West *Oklahoma State University*

Colorimetric biosensors are useful for early detection of viral infections as they are robust and simple. With the recent innovations in RNA-research, we aim to use nanoparticles conjugated with predetermined RNA sequences to detect multiple targets in a variety of biofluids. The focus of this study is how the nanoparticle-conjugates bind to their intended targets. This is a crucial part of this study, as it will provide a deeper understanding of how the calorimetric hybridization probes work. Each probe is made up of the respective RNA sequences of capture, target, and detection. Here we demonstrate the theoretical insights of possible hybridizations of RNA sequences present in a mixture of probes based on their binding energies and thermodynamic assembly. The direction of this research is to assess the binding mechanisms of multiple probes in a mixture through computational simulations to provide insights into the working mechanism of the sensor.

B64. Evaluation of Affordable Systems for Electrochemical Research

<u>Julio C Suarez</u>, Rachel Lewis, and Gabriel LeBlanc *University of Tulsa*

The high cost of electrochemical systems presents a significant barrier for researchers, with research-grade potentiostats and electrochemical cells often priced from hundreds to thousands of dollars. While these systems offer precise control and sensitivity for specialized applications,

many electrochemical experiments can be successfully conducted using far more affordable equipment. Previous studies have demonstrated the feasibility of using alkaline batteries and homemade devices for simple electrochemical investigations. In this work, we assess the effectiveness of low-cost power supplies and 3D-printed electrochemical cells as alternatives to traditional, high-cost setups. While these low-cost systems greatly reduce financial barriers to entry, we identify limitations, particularly in their performance in low-current applications. However, the flexibility of 3D printing enables the creation of custom electrochemical cells, offering distinct advantages in applications such as electrodeposition. We found that parameters like electrode positioning and electrolyte flow patterns are critical to the performance of these unconventional systems. Given their low cost and accessibility, we believe these systems can significantly broaden the adoption of electrochemical methods across a wider range of researchers and institutions.

B65. Green Synthesis of Silver Nanoparticles from Aqueous Clove Extract and their Antioxidant Activity

<u>Quentin Woodson</u> and Deshani Fernando *Mid-America Christian University*

The plant-mediated synthesis of silver nanoparticles (AgNPs) has gained considerable attention due to its cost-effectiveness and eco-friendly nature compared to conventional chemical and physical methods. Clove (Syzygium aromaticum) is a highly valued medicinal herb that is rich in phytochemicals, making it a promising natural resource for both biomedical applications and AgNP synthesis. However, a comprehensive understanding of the effects of key synthesis parameters (temperature, extract volume, reaction time, and pH) on the formation of AgNPs using aqueous clove extract remains limited. Therefore, this study systematically investigates the influence of these parameters on AgNP synthesis using ultraviolet-visible (UV-Vis) spectroscopy. The observation of the absorption band within the 425 nm- 440 nm range, as revealed by UV-Vis analysis, along with FTIR spectroscopy and TEM, confirmed the successful synthesis of AgNPs. Additionally, the antioxidant activity of AgNPs synthesized using clove extract was evaluated, highlighting their potential for future biomedical and environmental applications.

B66. 3D-Printed Electrodes Coated with Nickel Spray Paint for Hydrogen Gas Generation

Rachel M Lewis and Gabriel LeBlanc *University of Tulsa*

This research explored 3D-printed, nickel spray-painted electrodes for the purpose of efficient hydrogen gas generation. Cyclic voltammetry in sodium hydroxide (NaOH) electrolyte was used to evaluate the electrode's activity. Results revealed that the 3D-printed electrodes exhibited similar performance to nickel strip electrodes, with each generating approximately 6 mA of current. These findings suggest potential in effective hydrogen production, creating an inexpensive and accessible option to existing methods.

B67. Catalytic Transformation of Azide-Modified Gold Nanoparticles via Visible Light Activation for Biomedical Applications

Niloofar Valizadeh Dana, Mohadeseh Naderi, Shoukath Sulthana, Koie Kebert, Jimmie Weaver, and Yolanda Vasquez

Oklahoma State University

This study presents a novel method for functionalizing azide-modified gold nanoparticles using visible light-mediated photocatalysis. In this approach, Au-SH-PEG-N₃ is conjugated to folic acid via a photoclick reaction, with benzocycloheptene (BC7) serving as a linker. The reaction, carried out under blue LED illumination with an iridium-based photocatalyst, produces a triazoline click product, confirmed by NMR spectroscopy. During purification, the triazoline ring unexpectedly transforms into a stable triazole ring due to air oxidation, as verified by NMR, FTIR, and UV-Vis spectroscopy. This photocatalytic method offers several advantages over traditional approaches, including reduced toxicity, improved stability, and fewer side reactions. For biomedical evaluation, the functionalized nanoparticles were tested in RAW 264.7 macrophages. MTT assays showed low cytotoxicity in unstimulated cells and reduced viability in LPS-stimulated cells, suggesting potential anti-inflammatory effects and applications for targeted drug delivery. Ongoing studies will continue to explore biomedical potentials.

B68. In Silico and Enzyme Kinetic Evaluation of HMP-Alkyne as a Metallo-β-Lactamase Inhibitor

<u>Houa Thao</u> and Sean Kim Northeastern State University

Antibiotic-resistant bacteria threaten the effectiveness of known antibiotics, with metallo- β -lactamases (MBLs) emerging as major contributors to the failure of β -lactam antibiotics. These enzymes, particularly those from Bacillus anthracis, hydrolyze β -lactams and render them ineffective. MBLs require two zinc ions for catalytic activity, making zinc chelation an attractive therapeutic strategy. This study explores HMP-alkyne, a salicylic alcohol-containing compound, as an inhibitor of MBLs. In silico docking studies demonstrate favorable binding between the salicylic alcohol moiety of HMP-alkyne and the enzyme's active-site zinc ($\Delta G = -6.1$ kcal/mol). Enzyme kinetic analysis indicated that HMP-alkyne had a Ki value of 0.47 mM and an IC50 value of 0.161 mM, highlighting its affinity and strong inhibitory potency. The results also indicated that HMP-alkyne exhibits time-dependent inhibition. This study highlights the potential of HMP-alkyne to combat antibiotic resistance by restoring β -lactam efficacy through targeted MBL inhibition.

B69. Composition of Carbonaceous Aerosol from the Thermal Degradation of Plastics and Comparison to the Bulk Materials Using ATR-FTIR Spectroscopy

<u>Jace A. Barton</u>, Asma Soofi, and Elijah Schnitzler *Oklahoma State University*

Plastic incineration occurs widely around the world, and this process is a source of carbonaceous aerosol, which has an approximate lifetime of two weeks in the atmosphere. During this time, solar radiation and oxidants, like ozone, may age the particles, altering their chemical, physical, and optical properties. Consequently, it is important to study the composition and evolution of these particles. Here, we use a Fourier-transform infrared (FTIR) spectrometer with an attenuated total reflectance (ATR) crystal to investigate the composition of laboratory-generated carbonaceous aerosol from the thermal degradation of plastics and make comparisons to the bulk plastic materials. The aerosol samples are deposited on a glass fiber filter while heating a bulk plastic (e.g., polyethylene) in a quartz tube-furnace and then placed directly onto the ATR crystal.

This approach will help us better understand the origin and evolution of aerosol from plastic incineration and its potential effects on climate and health.

B70. Fe(OTf)3 or Blue Light Activated Diazo-Thioglycoside Donors for Stereoselective Glycosylations

<u>Adrienne Daroczi</u>, Umesh Chaudhary, and Surya Pratap Singh *University of Oklahoma*

Traditional methods for thioglycoside activation depend on expensive and toxic platinum-group metals. We present a catalytic glycosylation strategy utilizing diazo-thioglycoside donors, activated by earth-abundant iron or blue light without a photosensitizer. This approach exhibits orthogonal reactivity compared to conventional thioglycosides and alkyne-based donors, enabling one-pot glycan synthesis. The Thorpe-Ingold-like effect facilitates carbene proximity to sulfur, enhancing activation efficiency. This methodology supports various protecting groups and nucleophiles and applies to glycosyl donors such as glucose, mannose, galactose, rhamnose, xylose, lactose, 2-deoxyamino glucose, ribose, and arabinose. Additionally, it is effective for synthesizing challenging 1,2-cis furanosides, performing late-stage modifications on biomolecules like cholesterol and simvastatin at a gram scale, and enabling iterative hexasaccharide assembly. This sustainable strategy broadens the scope of glycosylation chemistry with practical and scalable applications.

B71. Artificial Photosynthesis and Recent Developments

Shantipriya Awasthi, Steven Otzoy, and Fazlur Rahman Oklahoma School of Science and Mathematics

This presentation will describe some useful developments in the field of artificial photosynthesis (AP). Using sunlight as catalysts, plants perform a useful simple chemical reaction resulting in a massive energy conversion turning 1200 billion tons of CO2 into carbohydrates (animal foods) every year. This process utilizes only 3% of the CO2 available in the earth's atmosphere. For the last three decades, the scientific community has been trying to develop a process (AP) to convert CO2 to fuel by mimicking the same energy system the plants do. Recent research results have shown that artificial photosynthesis can be beneficial for electrical power generators and reducing CO2 emissions. This presentation will describe recent technology developments in this emerging area by reviewing some recent scientific journal papers.

B72. Exploring Diphosphadisilatetrahedranes as Precursors for a Novel Zintl Anion

JP Sanza, and Mira Kessler Oklahoma State University

Zintl compounds, featuring polyanions formed by elements from group 14 to 17, exhibit fascinating structural diversity and thus find application in many areas, especially in materials science. Established synthetic strategies are typically so-called "top-down"

methods based on breaking down larger structures. However, these methods offer limited control over the size and composition of the resulting anions. In contrast, "bottom-up" strategies, which involve the systematic construction of Zintl compounds from smaller building blocks, enable precise control over cluster sizes and shapes but remain relatively uncommon. This study explores a novel synthetic approach towards binary Zintl anions by first constructing neutral, functionalized frameworks from molecular precursors and then selectively cleaving exocyclic bonds to the substituents. In particular, diphosphadisilatetrahedranes ($R_2Si_2P_2$) are investigated as potential precursors for the $[Si_2P_2]^{2^-}$ anion. A computational study on the stability of various $R_2Si_2P_2$ derivatives with different substituents (R) aims to identify promising candidates for synthesis.

B73. Combining Anharmonic Corrections with SQM Pulay Style Scale Factors to Improve Molecular Vibration Predictions

<u>JuHyeon Moon</u>, and William B. Collier *Oral Roberts University*

This research attempts to combine the best of two worlds in molecular vibration prediction. It is well known that LCAO-MO density functional calculated IR frequencies are systematically overestimated. One way is to correct computationally calculated IR and Raman spectra by a simple scale factor. Even better is to scale the calculated frequencies at the force constant level according to 12 functional groups or molecular bond types using the SQM Pulay method of scaling. The second method is to calculate the force field and resulting frequencies at a level beyond the traditional harmonic level. You add in the anharmonic frequency corrections. Only recently has it been possible to calculate anharmonic force fields and frequencies for sizable molecules using large scale parallelization on supercomputers. To combine the two methods requires compensation for the anharmonicity component present in Pulay scale factors. We present the results for carefully combining the two methods and explore the implications.

C1. Structural composites from post-consumer poly(ethylene terephthalate) (PET) carpet with recycled polypropylene (PP) resin

<u>Liyaqat Ali Kamran</u>, Mohamadreza Y. Azarfam, Aditya Nayar, Frank D. Blum, Ranji Vaidyanathan, Hadi Noori *Oklahoma State University*

Poly(ethylene terephthalate) (PET) and polypropylene (PP) are among the most widely used thermoplastics, commonly found in carpets and bottles. While many PET bottles are recycled most plastics generally end up in landfill sites as waste in the U.S. A method was developed to fabricate composites from post-consumer PET carpets (cPET) with recycled PP (rPP) resin using compression molding. However, making these composites is challenging since the polymers are dissimilar. Preliminary experiments were conducted to optimize the molding conditions. To evaluate the mechanical properties of these composites, particularly flexural strength and flexural modulus, three-point flexural bending tests were performed on the molded samples. Despite being composed of dissimilar polymers, these composites exhibited impressive flexural strength and modulus, indicating their potential use in structural applications. Optimized molding conditions

allowed these composites to have properties of structural materials. This research contributes to the reduction of post-consumer PET carpets in the waste stream.

C2. An Investigation of High Temperature Reactions Between Titanium, Silicon, and Yttrium Oxides

<u>Hunter Allen</u>, Dr. Dwight Myers *East Central University*

The objective of this research is to investigate and catalog how titanium and silicon oxides (TiO2, SiO2) react when a ternary (third) metal is introduced at high temperatures. Previous work in this group confirmed that TiO2 and SiO2 do not react with one another at high temperatures. It is well known however that adding a third metal oxide can initiate a reaction between titania and silica at high temperatures. One example is the reaction caused by adding calcium oxide to form titanite (CaTiSiO5). Our current ternary metal under investigation is yttrium. Other metals may be included in this study given an adequate time frame. Mixed oxide samples have been heated in a furnace at 1300 °C and 1400 °C. Sample characterization has been performed by X-ray diffraction. Results to date will be presented.

C3. NIR-II Photothermal Conversion by using Organic Cocrystals

Yuanning Feng

University of Oklahoma

I will introduce the recent research progress in our group. The first approach involves enhancing the near-infrared (NIR) absorption capacity by expanding the molecular π -conjugated systems or covalently linking electron donor-acceptor (D–A) fragments. The second approach aims to minimize radiative transition processes by increasing radical concentrations or enhancing the quenching effect.

C4. A Physical Approach to Protein Folding

<u>Pranav Domakonda</u>, Kidthusan Birendra Oklahoma School of Science and Mathematics

The formation of a protein's tertiary structure is crucial towards determining its function, as it establishes a 3-D conformation for biological activity. This study examines molecular forces that drive the tertiary structure formation. These forces depend on the individual amino acids that compose the polypeptide chain. Each amino acid has different chemical properties. For example amino acids such as leucine, valine, and phenylalanine are non polar, while amino acids such as tyrosine, threonine, and glycine are polar. The hydrophobic and hydrophilic portions of the protein are on the inside and outside respectively. The process of protein picks up from the secondary protein structure formation, including the formation of alpha helices and beta pleated sheets. The protein folding process continues through chemical interactions, including

hydrophobic interactions, hydrogen bonding, electrostatic interactions, and disulfide bridges. Our research will be on how the laws of physics shape these vital organic molecules.

C5. Characterization of an insect Pheromone Binding Protein: Implications for Environmentally Friendly Pest Management

<u>Pratikshya Paudel</u>, Omar Al Danoon, Shine Ayyappan, Smita Mohanty Oklahoma State University

The Asian corn borer (ACB), Ostrinia furnacalis (Lepidoptera: Crambidae), is a polyphagous agricultural pest that damages various crops across Asia, Australia, and Oceania. Current control methods largely depend on pesticides, which pose significant risks, including environmental pollution, human health hazards, pest resistance, and secondary pest outbreaks. Thus, there is an urgent need for controlling this invasive pest in an environmentally friendly and species-specific manner. ACB mating is mediated by female-emitted pheromones detected by males through Pheromone Binding Proteins (PBPs) in their antennae. Ostrinia furnacalis Pheromone Binding Protein 3 (OfurPBP3) is preferentially expressed in male antennae, binds and transports these hydrophobic pheromones to olfactory receptors, initiating olfaction. Structural and mechanistic studies of OfurPBP3 are essential to develop pheromone mimetics for effective pest management. This study presents the cloning, recombinant expression in E. coli, refolding from inclusion bodies, and characterization of OfurPBP3 using fluorescence spectroscopy, circular dichroism, and high-resolution solution NMR.

C6. The Evolution of Cancer Treatment: How Antibody-Drug Conjugates Are Changing Oncology

<u>Christina L. Dang</u> and <u>Julianne N. Hoang</u> *Oklahoma School of Science and Mathematics*

Traditional chemotherapy, while effective in treating cancer cells, often damages healthy cells, leading to severe side effects. However, recent advancements in targeted therapies—including small molecule inhibitors, monoclonal antibodies, antibody-drug conjugates (ADCs), and immunotherapy—offer improvements in the selectivity and effectiveness of cancer treatment by focusing on specific molecular targets. For example, ADCs release cytotoxic drugs inside the cancer cells to reduce damage to healthy tissues. Although targeted therapies in oncology have improved survival and side effects compared to conventional chemotherapy, some challenges include high costs, limited accessibility, and drug resistance and toxicity. Nevertheless, ongoing precision oncology research investigates the development of new targets and the simultaneous combination of multiple medications in combination therapy. Thus, this review summarizes the limitations of traditional chemotherapy, the impact of ADCs, and the challenges and future developments in precision oncology to further encourage a greater understanding and awareness of targeted therapies.

C7. Harnessing Mycoestrogens: Investigating Phallus impudicus for Estrogen

Receptor-Positive Breast Cancer

Anna E. Wilson, Dr. William P. Ranahan *Oral Roberts University*

This study investigates bioactive compounds produced by Phallus impudicus (common stinkhorn). P. impudicus is a medicinal mushroom historically used for treatment of hormone related cancers in women. Here we identify a compound which binds to the human estrogen receptor and results in cytotoxicity against estrogen receptor-positive (ER+) cancer cells. A cell viability assay was performed to assess cytotoxic effects on T-47D ER+ breast cancer cells, while an enzyme-linked immunosorbent assay (ELISA) was employed to detect estradiol-mimicking compounds. Preliminary findings suggest the presence of a novel mycoestrogen capable of binding to the human estrogen receptor, with ongoing research focusing on receptor phosphorylation and downstream gene expression. Additionally, cell viability assays have demonstrated significant cytotoxic effects on ER+ cancer cell lines. Future studies will compare effects on ER-positive versus ER-negative cell lines, expand investigations into ovarian and endometrial cancers, and further explore the therapeutic potential of mycoestrogens in women's health.

C8. Mesoporous Silica Beads

Resham Lal Shrestha

Oklahoma State University

High surface area mesoporous silica may be an efficient sorbent for treatment of organics in wastewater. The ability to reuse the sorbent makes sustainable material for treatments. To be effective, mesoporous silica needs to be formulated as mechanically robust beads in the mm range. The conversion of mesoporous silica powder into beads was performed using calcium alginate to form eco-friendly aqueous microreactors. The silica, along with a binding agent, was encapsulated in a calcium alginate bubble, where Ca2+ acts as a cross-linking agent. Binding agents include colloidal silica suspensions with different counter ions. Optimization of the preparation conditions and calcination temperatures provided 1 mm spherical beads with high surface areas (>200 m2/g), excellent thermal stability (>500°C) and mechanical strength. The synthesis of the mesoporous silica and the optimization of the beads will be discussed.

C9. Understanding and Managing Cholesterol Profiles: A Comprehensive Analysis of LDL and HDL Cholesterol Management

<u>Eunice S Kim</u>, Fazlur Rahman Oklahoma School Of Science and Mathematics

Cholesterol is essential for human health. Two main cholesterol components are low-density lipoprotein (LDL) and high-density lipoprotein (HDL) cholesterol. LDL, or "bad cholesterol," can build up in the walls of arteries, forming plaque. This build-up can lead to deadly heart

disease and stroke. HDL, or "good cholesterol," helps remove the LDL from the bloodstream and transports it to the liver to be broken down and eliminated from the body. Lifestyle modifications, such as healthy diets and regular exercise, are primary solutions for improving cholesterol levels. Additionally, medications such as PCSK9 inhibitors, which have been shown to lower LDL by inactivating proteins that regulate LDL levels in the liver, and Niacin, which increases HDL levels, have showcased significant improvements in cholesterol levels. However, these treatments may cause common side effects of muscle pain, back pain, and rashes. This study will explore the key benefits and risks of maintaining healthy cholesterol levels.

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Have a safe drive home, and thanks for attending the 2025 Oklahoma Pentasectional!