

American Chemical Society
Central Regional Meeting 2024

November 6 - 9, 2024
DoubleTree by Hilton - Green Tree
Pittsburgh, PA
acscerm2024.org

Program Book


54th Annual Central Regional Meeting (CERM) of the ACS
November 6 - 9, 2024
DoubleTree by Hilton - Green Tree | Pittsburgh, Pennsylvania

Organized by:
Pittsburgh Local Section of the American Chemical Society

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Welcome Letter from ACS President Mary Carroll

 CERM 2024 Welcome Letter.pdf

Organizers and Chairpersons

Matthew Price, General Co-Chair
PennWest University - California

Logan Miller, General Co-Chair
Shimadzu Scientific Instruments

Kevin Noonan, Program Co-Chair
Carnegie Mellon University

Kimberly Woznack, Program Co-Chair
PennWest University - California

Niharika Botcha, Treasurer
Carnegie Mellon University

Bradley Davis, Sponsorship Chair
Waynesburg University

Samuel Leung, Expo Co-Chair
Braskem

Brian Strohmeier, Expo Co-Chair

Alysia Mandato, Publicity Chair and Webmaster
University of Pittsburgh

Evonne Baldauff, Undergraduate Programming Chair
Waynesburg University

Edward Zovinka, Awards Chair
Saint Francis University

Karen Johnson, Activities Chair
NETL

Charnita Short, ACS Meeting Planner
ACS

Special thanks to other volunteers from the Pittsburgh ACS Local Section including Ronghong Lin, Kristin Nuzzio, Amalene Cooper-Morgan, and Toby Chapman.

CERM 2024 Sponsors



University of
Pittsburgh



MERCK



ACS Local Section
Pittsburgh



Oakwood
Chemical
Enabling Discovery



ACS Committee
International Activities



Huge thank you to all of our Sponsors and Exhibitors! We could not have done this without your support!

General Information

Registration

Onsite badge and registration materials can be picked up in the Grand Ballroom Foyer between 8 AM - 7:30 PM on Wednesday, 7 AM - 7:30 PM on Thursday, 7 AM - 7:30 PM on Friday, and 7 AM - 1:30 PM on Saturday.

Exposition Schedule

The Expo will be open on Thursday, November 7 from 9 AM - 5 PM and Friday, November 8 from 9 AM - 4:30 PM.

Lunch Options

There is an opportunity for a networking luncheon that can be added to your registration on Wednesday. Additionally, we have special topical group luncheons on Thursday and Friday. For lunch on-your-own, the hotel has the Champions Club restaurant. There is also a grab-and-go Bistro and Marketplace in the hotel open from 7 AM to 11 PM.

Coffee and Snack Breaks

Outside of the technical sessions, there will be morning and afternoon coffee and snack breaks included with your registration. Stop by to get a quick snack and chat with colleagues.

CERM 2024 Banquet and Awards Ceremony

On Thursday, November 7 at 6 PM, we will hold a cocktail hour prior to beginning the awards dinner and ceremony, where we will honor Pittsburgh and greater regional chemists.

Need Help?

Find an ACS staff member or a CERM volunteer wearing a volunteer ribbon on their name badge.

Program-at-a-Glance

Wednesday, November 6		
8 AM - 6 PM	Registration Opens	Lobby
9 AM - 12 PM 1 PM - 4 PM	Technical Program	Meeting Rooms
9 AM - 12 PM	Industry Workshops	Interstate or Salk Room
12 PM - 1 PM	Networking Luncheon	Westinghouse Room
1 PM - 3:30 PM	Brewery Workshop	PPG Room
4 PM - 5 PM	Sponsored Cocktail Hour	Green Tree Ballroom
5 PM - 6 PM	Plenary Lecture	Oakmont Ballroom
6 PM - 7:30 PM	Governance Reception	Green Tree Ballroom
8:30 - 9:30 PM	Glassblowing Demonstration	Off-site

Thursday, November 7		
8 AM - 6 PM	Registration Opens	Lobby
9 AM - 12 PM 1 PM - 4 PM	Technical Program	Meeting Rooms
9 AM - 5 PM	Expo Opens	Green Tree Ballroom
9 AM - 12 PM 1 PM - 4 PM	Industry Workshops	PPG Room
12 PM - 1:30 PM	Environmental Group Luncheon	Duquesne Room

4 PM - 5 PM	Poster Session	Green Tree Ballroom
5 PM - 6 PM	Plenary Lecture	Oakmont Ballroom
6 PM - 8 PM	Awards Dinner	Duquesne Room

Friday, November 8		
8 AM - 6 PM	Registration Opens	Lobby
9 AM - 12 PM 1 PM - 3:30 PM	Technical Program	Meeting Rooms
9 AM - 4:30 PM	Expo Opens	Green Tree Ballroom
9 AM - 12 PM	ACS Career Workshop	Interstate Room
12 PM - 1 PM	WCC Luncheon	Duquesne Room
1 PM - 3 PM	Resume Reviews	Interstate Room
1 PM - 5 PM	SMID-DEIR Workshop	Ohio Room
3:30 PM - 5 PM	Poster Session	Green Tree Ballroom
4:30 PM - 6 PM	Undergraduate Reception	Duquesne Room
6 PM - 7 PM	Plenary Lecture	Oakmont Ballroom

Saturday, November 9		
8:30 AM - 9:30 AM 2 PM - 4 PM	Student Research Presentations	Heinz Room

Exhibitors and Expo Map

MilliPore Sigma

Booth #101

<https://www.sigmaaldrich.com/US/en>**Oakwood Chemical**

Booth #103

<http://oakwoodchemical.com/>**Nanalysis Corp.**

Booth #105

<https://www.nanalysis.com/>**GlycoSurf, Inc.**

Booth #107

www.glycosurf.com**Merck**

Booth #109

<https://www.merck.com/>**Across International LLC**

Booth #111

<https://www.acrossinternational.com/>**JASCO, Inc.**

Booth #113

<http://jascoinc.com/>**Agilent Technologies**

Booth #115

<https://www.agilent.com/>**University of Pittsburgh**

Booth #117

<https://www.chem.pitt.edu/>**Shimadzu Scientific Instruments**

Booth #102

<https://www.ssi.shimadzu.com/>**Bettersize Inc.**

Booth #104

www.bettersizeinstruments.com**Florida State University**

Booth #106

<https://www.fsu.edu/>**Vernier Science Education**

Booth #108

<http://www.vernier.com/>**Magritek**

Booth #110

<https://magritek.com/>**ACS Marketing**

Booth #112

<https://www.acs.org/>**SACP/SSP**

Booth #114

<https://chemistryoutreach.org/>**Bruker**

Booth #116

<https://www.bruker.com/en.html>**Velp Scientific, Inc.**

Booth #118

<https://www.velp.com/>

Swagelok Pittsburgh

Booth #119

<https://pittsburgh.swagelok.com/en>**Axcend**

Booth #120

PPG

Table #201

<https://www.ppg.com/en-US>**Analytik Jena**

Table #203

<https://www.analytik-jena.us/>**Ohio University**

Table #205

<https://www.ohio.edu/engineering/chemical>**ICSPI (AFM Instruments)**

Table #207

<https://www.icspicorp.com/>**Pittsburgh Section of the ACS**

Table #202

<https://pittsburghacs.org/>**RoCo, Liquid Ion Solutions LLC**

Table #204

<https://roco.global/>**ACS Senior Chemists Committee**

Table #206

<https://www.acs.org/content/acs/en/membership-and-networks/senior-chemists.html>**University of Pittsburgh/CMU****Molecular Biophysics and Structural Biology**

Table #208

<https://www.mbsb.pitt.edu/>

Technical Program Schedule

Wednesday Oral Sessions

Thompson Room

Advances in Renewable Energy and Sustainability

S. Goswami, S. Talledo, J. Vinskus, *Presiding*

9:00 Opening Remarks.

9:05 1. Coupling CO₂ capture and conversion to CH₄. **T. Neves-Garcia**, M. Hasan, Q. Zhu, J. Li, Z. Jiang, Y. Liang, H. Wang, L.M. Rossi, R. Warburton, L. Baker

9:25 2. Revisiting concepts of nucleation and growth in multimetallic nanoparticles. **J. Millstone**

9:45 3. Ring-opening metathesis polymerization toward donor-acceptor conjugated polymers. **B.C. Bickerton**, K. Pasquarella, S. Koehler, K. Hauer, J. Lin, E. Elacqua

10:05 4. Effect of polymer composition on performance for norbornene based anion exchange membranes. **C. Birch**, J. Gaitor, T. Kowalewski, K.J. Noonan

10:25 Intermission.

10:40 5. Mass spectrometry in advancing the use of renewable feedstocks for sustainable energy. **H.I. Kenttamaa**

11:00 6. New cyclometalated Co(III) complex exhibiting picosecond metal/ligand-to-ligand charge transfer states. **S. Burton**, G. Lee, C. Turro

11:20 7. Enhancing the electrocatalytic CO₂ reduction using imidazolium-based ionic liquids in the presence of external magnetic field. **N. Karki**, A. Wilson

11:40 8. Nanostructured materials for advanced rechargeable batteries. **M.M. Kaid**, H.M. El-Kaderi

Mellon Room

General Environmental Chemistry

C. A. McDonough, R. C. Sullivan, *Organizers, Presiding*

9:00 9. Mechanistic studies of thermo-catalytic defluorination of PFAS compounds using TGA-IR-GC/MS integrated system. **A. Tegenaw**, E. Sahle-Demessie, B. Mezgebe, Y. Shan, M. DeSantis

9:20 10. Nontarget analysis of transformation products from droplet-accelerated photo-oxidation of per- and polyfluoroalkyl substances (PFAS) using Chemical ionization mass spectrometry (CIMS). **R. Weatherholt**, B. Bowers, K. Chung, G. Thornhill, N. Bhattacharyya, R.C. Sullivan

9:40 11. High-resolution mass spectrometry and advanced separation methods for understanding PFAS bioaccumulation. **K.E. Hon**, D. Perera, C.A. McDonough

10:00 12. Analytical strategies for a more complete picture of total PFAS burden in environmental and biological samples. R. Smolinski, D. Perera, D. Dukes, **C.A. McDonough**

10:30 Break.

10:50 13. *Ex-situ* passive sampling to understand the bioavailability of per- and polyfluoroalkyl substances (PFASs) in contaminated marine sediments. **L. Mukhopadhyay**, M. Laney, A. Zhao, J. Becanova, C.A. McDonough

11:10 14. Statin contamination, bioaccumulation and fate in aquatic habitats: An investigation of wastewater effluent effects. **D. Sanchez**, G. Kotchey, J. Kingsbury

11:40 15. Experimental and computational studies on the toxicity of mefenpyr diethyl safener to *D. magna*. **O. Femi-Oloye**, F.F. Oloye, J.P. Giesy

Ohio Room

General Materials Chemistry

K. J. Noonan, *Organizer, Presiding*

9:00 16. Predictive incremental tuning of metal-organic framework color and quantum yield with post synthetic modification. **Z. Soilis**, J. Brennan, T. Choi, K. Johnson, R.R. Frontiera, N.L. Rosi

9:20 17. Withdrawn

9:40 18. Interactions of DNA Origami with silane based Self-Assembled Monolayers (SAMs). **S. Kundu**, S.P. Moore, A. Kumari, H. Liu

10:00 19. Multimetallic Metalorganic framework for electrochemical detection of 4-aminophenol and environmental applications. **V. Yempally**, D. N, A. Gupta, A. M. U, H. Kaur

10:20 Intermission.

10:35 20. Tale of two polymorphs: linear and non-linear optical properties of uniaxial and biaxial diamond-like polymorphs of $\text{Cu}_2\text{ZnGeS}_4$. **J.A. Aitken**, J. Kelly, J. Jang, Z. Messegee, X. Tan, C.E. Hoyer, J. Chase

11:00 21. Tuning the length and stability of single helical gold nanoparticle assemblies. **Y. Zhang**, Y. Zhou, S. Brooks, N.L. Rosi

11:20 22. Tailoring reaction kinetics to direct structural outcomes in bimetallic nanoparticles. **J. Smith**, J. Millstone

11:40 23. Influence of surface chemistry on metal deposition outcomes in copper selenide-based Nanoheterostructure synthesis. **S. Millheim**, R. Sen, T.M. Gordon

Heinz Room

Inorganic Chemistry/Catalysis

B. Dolinar, B. V. Popp, *Organizers, Presiding*

9:00 24. Hydrofunctionalization studies of terminal alkenes with a Tridentate Pincer-Ligated Fe^{II} catalyst. **C. Nieto**, C.M. Thomas

9:20 25. Rhodium(I)-catalyzed regioselective [2+2+2] cyclootrimerization of tethered 1,6-diynes. **N. Selvaraj**, B.V. Popp, G.B. Dudley

9:40 26. Nickel-catalyzed cyclootrimerization of terminal alkynes with vinyl sulfone. **E.L. Heller**, S.M. Long, G.B. Dudley, B.V. Popp

10:00 27. Synthesis of constrained diphosphine ligands and their Fe and Co bis-chelate complexes. **L. Wolff**, C.R. Wade

10:20 28. Ligand-controlled selective couplings of organotetrafluorosilicate and aryldiazonium salts. **D. Dugger**, C. Stultz, M. Lange, R. Van Hoveln

10:40 Intermission.

10:50 29. Enhanced PCET reactivity by a mononuclear NiOH radical complex. **D. Ye**, I. Garcia-Bosch

11:10 30. Unquenched orbital angular momentum in non-linear two-coordinate transition metal complexes: Synthesis, magnetic properties, and potential single-molecule magnetism. **S. Noor**, B. Dolinar

11:30 31. Bond dissociation free energy of an O-H bond in a Zr/Co heterobimetallic complex measured by open-circuit potential. **J. Feresin**, B. Barden, J. Reyes, S. Barrett, C.M. Thomas

11:50 32. Synthesis and characterization of Zr metal-organic cages with P₂N₂ linkers. **J. Shin**, C.R. Wade

Frick Room

General Analytical Chemistry

A. Mandato, *Organizer*

10:50 Introductory Remarks.

11:00 33. New convenient method to assess antibiotic resistance and antimicrobial efficacy against Pathogenic *Clostridioides difficile* Biofilms. **L. Xu**, B. Gurung, C. Gu, S. Wang, T. Gu

11:20 34. Cytosolic chloride indicators for real-time chloride imaging in live cells.
K. Leung

11:40 35. Heterogeneous non-canonical inflammasome LPS-mediated oligomerization probed by electron capture charge reduction mass spectrometry.
P. Lacey, C. Wang, J. Ruan, V.H. Wysocki

Thompson Room

Advances in Renewable Energy and Sustainability

S. Goswami, S. Talledo, J. Vinskus, *Presiding*

1:00 Opening Remarks.

1:05 36. High throughput methodology for investigating green hydrogen generating processes using colorimetric detection films and machine vision. **S. Talledo**, A. Kubaney, M. Baumer, K. Pietrak, S. Bernhard

1:25 37. Harnessing electrolytic hydrogen for decarbonized chemical manufacturing. **J.R. McKone**

1:45 38. Polymer-based photoredox catalysts: synthesis, characterization and applications. **S. Gaikwad**, M. Spicuzza, S. Baldwin, E. Elacqua

2:05 39. Current advancements of Potassium-Air batteries. L. Qin, L. Schkeryantz, **J. Elgin**, Y. Wu, J. Sun, J. Zheng

2:25 Intermission.

2:40 40. Toward high entropy catalyst libraries that minimize precious metal content. **R.E. Schaak**

3:00 41. Potassium-ion based water-in-Bisalt electrolyte with hydrophilic and hydrophobic anions. **M. Dhasarathaboopathy**

3:20 42. Enhancing photoelectrochemical performance for water splitting through graphene composite materials. **Y.A. Sirina**

3:40 43. Photopolymerization of pyrrole thin films. **A. Portaro**, W.R. Lowery, D.E. Cliffl

Frick Room

General Analytical Chemistry

A. Mandato, *Organizer, Presiding*

1:00 44. Withdrawn

1:20 45. Identifying the chemical composition of kombucha tea. **G. Garza**, G. Ryser, J.L. Sarver

1:40 46. Identification of the degradation products of moxidectin by HRMS and NMR, and HPLC method optimization of impurity analysis. **T.C. Huang**, Y. An, J. Gao, F. Rinaldi

2:00 Intermission.

2:20 47. Essential leadership practices for creating and maintaining successful analytical laboratories. **B.R. Strohmeier**

2:40 48. Self-ionizing e-cigarettes enable direct vape analysis via mass spectrometry. **N.C. Auvil**, M.E. Bier

3:00 49. Withdrawn

3:20 50. Highly sensitive early detection of chronic traumatic encephalopathy biomarkers using nonlinear multi-photon laser wave-mixing spectroscopy. **N. Shatirishvili**

Mellon Room

General Environmental Chemistry

C. A. McDonough, R. C. Sullivan, *Organizers, Presiding*

1:00 51. Autooxidation of nitrous acid to nitric acid in supermicron aqueous droplets is acid accelerated. L. Monroe, J. Hall, G. Thornhill, **R.C. Sullivan**

1:30 52. Computational model for the degradation of fulvic acid. **M. Martin**, L. Tribe

1:50 53. Determining the role of aerosol acidity and buffering capacity in the reactive uptake and chemical feedbacks of gaseous N_2O_5 -organic aerosol systems. **G. Thornhill**, L. Monroe, J. Hall, R. Sullivan

2:10 Break.

2:30 54. Ion-lipid binding and water at proxy Ocean and aerosol aqueous surfaces. **H.C. Allen**

3:00 55. Expanding the green-chemical toolbox: development of improved dioxygenase catalysts through enzyme engineering. **J. Froese**

3:20 56. La@MOF-808: a multifunctional adsorbent for simultaneous removal of arsenic and lead from water. D. Sanchez, **H. Nawaz**

3:40 Discussion.

Ohio Room

General Materials Chemistry

K. J. Noonan, *Presiding*

1:00 57. Consumer plastic waste upcycling into graphitic carbons: Characterization and mechanism(s). **R.L. Vander Wal**, A. Gharpure, M. Kowalik, A. van Duin

1:20 58. Metal-organic framework dienophile scaffolds for controlling Diels-Alder diastereoselectivity. **S. Yannucci**, N.L. Rosi

1:40 59. Ligand-based approach for the design, synthesis, and control of dimensionality of rod-based MOFs. **G. He**, N.L. Rosi

2:00 60. Continuous nucleation of metallic nanoparticles *via* photocatalytic reduction. **A. Paterno**, Z. Simon, J. Millstone

2:20 Intermission.

2:40 61. Withdrawn

3:00 62. Exploring the nanoscale and macroscale electromechanical response of self-assembled monolayers. **C. Chun**, G. Hutchison

3:20 63. Calculations-based methods as predictors for candidate infrared nonlinear optical (IR-NLO) materials. **K.E. Colbaugh**, J.A. Aitken

3:40 64. Unraveled the influence morphologies of freestanding Pd nanocrystals and electrolytes on ethanol oxidation electrocatalysis. **A.M. Abdullah**, A.K. Ipadeola, B. Salah, K. Eid

Heinz Room

Inorganic Chemistry/Catalysis

B. Dolinar, B. V. Popp, *Organizers, Presiding*

1:10 65. Enzymatic $[4\text{Fe-4S}]^+$ intermediate with $S = 7/2$ ground state in the archetype of group 4 ferredoxin: Thioredoxin reductase. **J. Xiong**, A. Rai, J.G. Ferry, D. Prakash, E.L. Bominaar, Y. Guo

1:30 66. Mechanistic Investigation of a Non-Heme Iron Halogenase involved in the biosynthesis of 2'-Cl-2'-dAMP. **P. Palacios**, Y. Guo, W. Chang

1:50 67. Effect of surface oxygen vacancy and morphology on photoelectrocatalytic efficiency of CuO/TiO₂-based thin film heterostructures. A. Patnaik, **S. Das**, L. Baker

2:10 68. Synthesis, characterization reactivity of bionspired NiFe H₂ase model complexes using tetradentate bis(amide)bis(phosphine) ligand. **J. Fletcher**, C.M. Thomas

2:30 69. Metal-ligand orbital energy match for the proton coupled electron transfer reactions in transuranic high valent species. **C. Studvick**, K.S. Otte, J. Niklas, H.S. La Pierre, I.A. Popov

2:50 Intermission.

3:00 70. Tuning peripheral metal-ligand interactions in a series of quasi-linear two-coordinate transition metal complexes with sterically bulky carbazole ligands. **B.S. Dolinar**

3:20 71. Copper-catalyzed cross coupling approaches to selective PTM modifications. **Z.T. Ball**

3:40 72. Solid-state ligand design and catalysis using metal-organic frameworks. **C.R. Wade**, J. Hilliard, A. Greene

4:00 73. Heterobimetallic Zr(IV)/Co(I) catalyzed dinitrogen binding and catalytic silylation under ambient reaction conditions. **A. Singh**

Plenary 1

K. J. Noonan, K. A. Woznack, *Organizers*

5:00 74. Macromolecular Engineering by Atom Transfer Radical Polymerization. **K. Matyjaszewski**

Thursday Oral Sessions

Salk Room

S-STEM: Goals, Best Practices for Success, and Scholars' Experiences

A. Cooper-Morgan, *Organizer*

H. Juzwa, *Presiding*

8:50 Opening Remarks.

9:00 75. Anecdotes of a current NSF S-STEM Scholars Program from a professor's point of view. **A. Cooper-Morgan**

9:20 76. Anecdotes of a current NSF S-STEM program from students' point of view. A. Cooper-Morgan, **T. Gould, J. Sobotka, N. Saloom, P. Cercone**, N. McAllister, A.L. Bartelson

9:50 77. Chemical laboratory technician training model. **K. Weiler**, K. Rassau

10:20 Intermission.

10:30 78. Helping students explore and build positive STEM identities: An interdisciplinary cohort design. **J.R. Boothe**, O.S. Long, K.A. Heffernan, B.J. Barnhart, J. Ingram

11:00 79. Lessons learned from the STAR NSF S-STEM grant. **J. Novak**, P. Tandler, M.J. Dunphy

11:30 80. Perspectives from four NSF S-STEM Awards for Engineering and Computing Studies at Gannon University. **K.M. Vernaza**

Mellon Room

Carbon Materials and Their Applications

R. Lin, *Organizer, Presiding*

H. Liu, *Presiding*

9:00 81. Cell-instructive peptide-graphene oxide conjugates for improved bone regrowth and vascularization. **M.E. Wolf**

9:20 82. Synthetic bone grafts with antibacterial and osteoinductive properties derived from polylysine functionalized calcium phosphate graphene. **J. Orlando**

9:40 83. Molecular dynamics simulations of 2D-layered graphene sheets with tandem repeat proteins. **O. Colak**, A. Nicolaï, V. Meunier, M.C. Demirel

10:00 84. Biosensing with carbon nanotube-based field-effect transistors. **A. Star**

10:30 Coffee Break.

10:45 85. Wetting transparency of single-layer graphene on liquid substrates. **L. Li**, H. Liu

11:15 86. Tunable fluorescent quantum defects on carbon nanotubes. **B. Heppe**, X. Sun, G. Ao

11:45 87. Unveiling the structural parameters of graphitic and non-graphitic carbons derived from biopitch precursors. **B. ANTIL**, R.L. Vander Wal

Ohio Room

General Materials Chemistry and Chemistry Education

K. J. Noonan, *Organizer*

E. P. Zovinka, *Presiding*

9:00 88. Delivery of a protein-based cellular growth factor by a zinc-coordinating self-assembling peptide hydrogel. **B. Clegg**, G. Reddy, K. Velankar, W. Meng, E.S. Gawalt

9:20 89. Derivatization using post synthetic exchange in multicomponent imidazolite metal-organic frameworks. **N.T. Garrett**, L.P. Moore, M.H. Mohamed, N.L. Rosi

9:40 90. Withdrawn

10:00 91. Octadecane-poly(ethylene glycol)-octadecane material as a delivery platform for retinal gene therapies. **J. Westbay**, M. DiLeo, L. Byrne, J. Sahel, W. Beltran

10:20 Intermission.

10:40 92. Solid Stuff: Using materials science to engage and excite secondary and college chemistry student. **J. Sickles**

11:00 93. Bringing metals chemistry back to the general chemistry teaching lab: How to create bismuth-tin eutectic alloys. **M.A. Benvenuto**, H. Song, R. Nistor, M. Naddaf, U. Fargo, S. Thouraya, L. Jeki

11:20 94. Organic chemistry laboratory for a summer high school program adapted from the undergraduate organic chemistry laboratory course at Carnegie Mellon University. **N. Botcha**

11:40 95. Incorporating green chemistry into inorganic chemistry courses. G. Ross, J. Koval, j. dee, **E.P. Zovinka**

Frick Room

General Physical Chemistry

A. Konar, *Organizer*

J. D. Shipp, *Presiding*

9:00 96. Functionalization of nitrogen vacancy-containing nanodiamonds with a metal-organic framework for quantum sensing applications. **S. Crawford**, R. Shugayev, J.P. Baltrus, N. Diemler, J. Ellis, K. Kim, Y. Duan

9:20 97. Spectroelectrochemistry of helical polyfurans: Elucidating the impact of structure. **S. Westrey**, D. Sharma, Y. Shang, T. Kowalewski, K.J. Noonan, L.A. Peteanu

9:40 98. Ultrafast circular dichroism spectroscopy: Observing spin polarized electron dynamics in chiral metal oxides. **A. Partin**, C. Dykstra, H. Gajapathy, L. Baker

10:00 99. Hydronium ions are less excluded from hydrophobic polymer interfaces than hydroxide ions. **R. Myers**, A. Taira, C. Yan, S. Lee, L. Welsh, P. Ianaro, T. Yang, K. Koga, P.S. Cremer

10:20 Break.

10:40 100. Effect of partitioning on the heterogeneous oxidation of multi-component aqueous aerosols. **K. Selvaraj**, T. Masaya, F. Goulay

11:00 101. Multispectral multidimensional spectroscopy reveals charge transfer in the red sites of cyanobacterial Photosystem I. **J.D. Shipp**, C. Li, Y. Lee, M. Gorka, J. Golbeck, J. Anna

11:20 102. Proton transfer Equilibria in nonstoichiometric Pseudoprotic Ionic liquids. **M.N. Kobrak**

11:40 103. Synthesis and characterization of catalyst loaded silica gel beads using droplet microfluidic techniques. **K.B. Shumba**, M. Tinsley, S. Nkomo, K. Showalter

Interstate Room

Polymer Chemistry and Circular Carbon

S. Leung, *Organizer, Presiding*

V. Vargheese, *Presiding*

9:00 Introductory Remarks.

9:05 104. Synthesis and investigations into chemical recycling of disulfide containing polyethylene. **J. Vinskus**, K.J. Noonan, C. Birch

9:25 105. Hydrocracking of PVC-mixed polyolefin (PO) over Bifunctional tungsten-carbide (W_xC) catalysts. U. Nwachukwu, M. Moegling, S. Pere, M.D. Porosoff, **L. Chen**

9:45 106. Microwave-assisted processing of single use plastic waste for circular economy. **A.S. Gowda**

10:05 107. Precision control of size, tacticity, and chirality in ultra-high molecular weight bottlebrush polymers via Photoiniferter polymerization for biomacromolecule mimicry. **L. Trachsel**, J.D. Hillman, F. De Luca Bossa, B.S. Sumerlin, K. Matyjaszewski

10:25 Intermission.

10:40 108. Proteins as reinforcing components in copolymers and composites. A.E. Ashmar, S. Surprenant, **W. Chan**

11:05 109. Selective depolymerization of thermoplastic polyurethane: Turning limitations into an opportunity. R. Rafiq, H. Zucco, D. Sheppard, J. Plusnin, M. Persoons, G. Cormack, **G. Veser**

11:25 110. Realizing end-of-life Poly-olefinic circularity: A commentary on commercial challenges and opportunities of continuous recycling of molecules. **S. Cotts**

11:45 111. Enhancing recycling and upcycling of polymers with reactive ionic liquids. **H.B. Nulwala**

Thompson Room

Thin Films: Fabrication and Applications

S. Crawford, *Organizer, Presiding*

9:00 112. Mechanoactivated shape-morphing and origami by exploiting plasticity in multilayered thin films. C. Nguyen, K. Ramalingam, Z. Kushnir, F. Rouhani, **S. Velankar**

9:35 113. Functionalized imidazolium ionic liquids for the interfacial defect passivation of perovskite solar cells. **R. Panta**, C. Grapperhaus, T. Druffel

9:55 114. Liquid metal: Polymer composite films for soft electronics and thermal management. **C. Majidi**

10:30 115. Hf-doping of polycrystalline gallium oxide thin films. **S.E. Chamberlin**, S.T. King

10:55 116. Optical wavefront distortion analysis: Applications to chemical sensors. **D.M. Snyder**

11:20 117. Beam plasma source enhanced thin-film growth at low temperatures. **Q.H. Fan**

Salk Room

Diversity, Equity, Inclusion, and Respect (DEIR) in Chemistry

K. A. Woznack, *Organizer, Presiding*

1:00 Opening Remarks.

1:05 118. Mapping my journey: My evolving path to understanding and embracing diversity and inclusion. **A.F. Charlebois**

1:25 119. Seton Hill's future scholars program: A STEM equity program. **S.L. Joiner**, D. Haworth-Ward, **A. Cooper-Morgan**

1:45 120. Building on a solid past to excel in an uncertain future. **L. Tribe**

2:05 121. Senior chemists committee's efforts to promote DEIR. K.M. Kallury, M. Orna, J.A. Obaleye, **F. Butwin**, L.W. Hoffman, V.J. Kuck, M. Levenberg, L.J. Berliner, R.A. Yokley

2:25 122. Fitting students for the scientific world in which they will work: Embedding career development across the chemistry curriculum. **D.K. Hoover**

2:45 Intermission.

3:00 123. What's your Superpower? Unique life experience creates positive impact. **M.R. Cummings**

3:20 124. Facilitating an inclusive environment in the technical workplace. S. Leung, **D.D. Hess**, L. Li, R.S. Caulkins

3:40 125. Elevating professionalism through the power of diversity equity inclusion and respect. **J. Cohen**

4:00 126. LSAC and local sections promoting Diversity, equity, inclusion and respect (DEIR). **B.A. Lorsbach**

Frick Room

General Physical Chemistry

A. Konar, *Organizer, Presiding*

1:00 127. Computational chemistry in the classroom: Introducing molecular dynamics simulations at the undergraduate level. **J.L. Sarver**

1:20 128. First principles investigation on CO and H co-adsorption on Pt (111) surface using multisite multi-adsorbate cluster expansions. **S. Hossain**, R.B. Getman

1:40 129. Theoretical study of the gas phase reaction of OH radical with cyclopentenone derivatives. **E.I. Ubana**, P. Rutto, F. Goulay

2:00 130. Natural bond orbital (NBO) analysis of the nature of copper-halogen bond in transition metal complexes used in atom transfer radical polymerization (ATRP). **L. Madureira**, J. Sobieski, K. Matyjaszewski, T. Kowalewski

2:20 Break.

2:40 131. α -Ketoglutarate-dependent non-heme iron enzyme HrmJ and homolog reaction pathways: A molecular dynamics study. **S. Koby**, I. Kurnikov, Y. Guo, W. Chang, M.G. Kurnikova

3:00 132. Benchmark all-atom and coarse-grained force fields for simulating the K18 form of the intrinsically disordered protein tau. **X. He**, V.H. Man, J. Wang

3:20 133. β -Keto acid decarboxylation: Microsolvation determines conformation and energetics of uncatalyzed monoanionic malonate decarboxylation. **U. Puthumana**, A. Tamez, L. Andreola, I. Pathiraja, K. Jemison, J. Rohde, D.J. Fox, J.D. Evanseck

3:40 134. Toward a better understanding of Ni coarsening in solid oxide cells: NiH on Ni (111) examined at the level of density-functional theory. **Y.A. Mantz**, Y. Lei, W.A. Saidi

Ohio Room

Main Group Chemistry in the 21st Century and General Organic

P. Lummis, *Organizer*

K. J. Noonan, *Presiding*

1:00 275. N-Heterocyclic carbene complexes of the s-block metals. **P. Lummis**, D. Bedillion, A.M. Banks, J. Kelly

1:25 276. Intrinsic reactivity of discrete organometallic group II cations measured using ion trap mass spectrometry and computational chemistry. **M. Van Stipdonk**, L. Metzler, T.A. Corcovilos

1:45 277. Alkaline stable tetraaminophosphonium cations appended to polyolefin backbones for anion-exchange membranes. **K.J. Noonan**

2:05 278. Highly alkaline stable novel phase transfer catalysts derived from proazaphosphatranes. **C. Birch**, N. Fisherman, Y. Wang, J. Vinskus, T. Kowalewski, K.J. Noonan

2:25 Intermission.

2:45 279. Development of BODIPY-based functional fluorophores for subcellular imaging. **K. Leung**

3:05 280. Synthesis of 2,3,4-trisubstituted tetrahydroquinolines and their development as novel K_v7 channel agonists. **C. Hill**, P. Wipf

3:25 281. Effect of donor group positionality on the brightness and stability of donor-acceptor near-IR fluorescent dyes. **M. Ghazala**, S.P. Garcia, S. Moaven, C. Sheldon, D.L. Watkins, C. Turro

3:45 282. Green extraction of wheat phenolic compounds using microwave-assisted extraction (MAE). **R. Nandasiri**, K. Kirusnaruban, N. Gasparre, C. Rosell

Heinz Room

Nucleic Acid Chemistry

B. A. Armitage, X. Tan, D. Yang, *Presiding*

1:00 Introductory Remarks.

1:05 135. Host immune microRNA interactions with the SARS-CoV-2 viral genome 3'-untranslated region. **C.J. Frye**, C. Cunningham, D. Heisler, M. Mihailescu

1:25 136. Bending unwinds DNA. S. Chandrasekhar, S. Thomas, D. Hollis, F. Fadaei, R. Bricker, D. Houser, J. Portman, **T.L. Schmidt**

1:50 137. HIV-1 DIS atomistic transition pathway from kissing complex to extended duplex. **J.A. Makowski**, A. Kensinger, M. Mihailescu, J.D. Evanseck

2:10 138. Unlocking efficiency: Native circular surpass linear isoforms in RNase P activity. **A.K. Chawla**, A.M. Kietrys

2:30 Coffee Break.

2:40 139. Hidden links: Nucleobase protonation in riboregulators and implications for RNA-targeted drug discovery. M. Hossain, O. Fatunbi, D. Herath, D. Amesaki, E. Murphy, **J.V. Hines**

3:05 140. Withdrawn

3:25 141. TERRA Illuminata: Imaging of telomeric RNA using fluorescent gammaPNA miniprobos. R. Dalath, M. Riley, M. Xu, N. Hasija, H. Zhang, **B.A. Armitage**

Thompson Room

Thin Films: Fabrication and Applications

S. Crawford, Organizer, Presiding

1:00 142. Fabrication of metal-organic framework thin films for luminescent sensing applications. **S. Crawford**, K. Kim, C. Adams, J. Ellis, J.P. Baltrus

1:35 143. Multi-layer films for structural coloration. **P. Leu**, J. Kim, S. Iyengar, O. Hinder

2:10 144. Withdrawn

2:45 145. Investigation of post-polymerization modifications on the morphology and antimicrobial performance of anionic multi-block polymer thin films. **F.E. McFeaters**, R.A. Ghiladi, R.J. Spontak

3:05 146. Thin film synthesis of highly metastable oxide polymorphs using combinatorial substrate epitaxy and interval pulsed laser deposition. C. Zhou, G.S. Rohrer, **P. Salvador**

Mellon Room

Carbon Materials and Their Applications

R. Lin, *Organizer, Presiding*

H. Liu, *Presiding*

1:10 147. Toward greener synthesis of activated carbons. **M. Marszewski**, R. Bamidele

1:30 148. Laser-induced graphene: Factors governing synthesis and potential applications. **M. Bedewy**

1:55 149. Heteroatom doping of graphitic carbon nitride: Investigating correlations with environmental impact of syntheses and photocatalytic reactive species production. **Y. Shah**, L.M. Gilbertson

2:20 150. Upcycling polyethylene waste to advanced carbon materials for energy storage applications. **Y. Gao**, N. Huynh, V. Pham, C. Wang, C. Matranga, K. Kim

2:45 Intermission.

2:55 151. Granular activated carbon (GAC) for PFAS removal and destruction: A full-scale reactivation study. **R. Distefano**, T. Knowlton, M. O'Brien

3:20 152. Microstructural analysis of Metal-embedded carbon molecular sieve (CMS) membranes for sustainable ammonia synthesis. **N.H. Khuu**, J.M. Harrah, B.K. Desta, M.M. Kulkarni, M. Ball, J. Hu, O. SANYAL

3:40 153. Self-supported carbon nanofibers derived from linear polyethylene precursors as potential CO₂ adsorbents. **R. Garduque**, J. Wang

Interstate Room

Polymer Chemistry and Circular Carbon

S. Leung, *Organizer, Presiding*

S. Dwivedi, *Presiding*

1:10 154. Liquids that freeze when mixed: Thermodynamics and kinetics of co-crystallization of polyoxacyclobutane with water. **S. Velankar**, S. Banerjee, E. Barker, T.Y. Meyer

1:30 155. Novel conjugated electronic materials with a twist: Design, synthesis, and characterization of furan-based macrocycles and helical polymers. **D. Sharma**, K.J. Noonan, T. Kowalewski, L. Peteanu

1:50 156. Esterified protein fibrils serve as fibrous reinforcing agents in polymer composites. **A.E. Ashmar**, W. Chan

2:10 157. Synthetic polypeptide-enhanced injectable hydrogels for cartilage regeneration. **J. Singh**, J. Kadir, S.A. Sydlik

2:30 Intermission.

2:50 158. Emerging technique sees microdynamics in carbon dioxide based polycarbonate vitrimers. **S. Aracri**, S. Joshi, S. Yoon, J.M. Eagan, J. Wang, M.D. Foster

3:10 159. Enhancing UV stability in pigment dispersions using Hals-functionalized acrylic dispersants. **S.E. Bowles**

3:30 160. Covalent adaptive networks for protein-based elastomers. **S. Surprenant**, W. Chan

3:50 161. Incorporation of dynamic covalent bonds in polymerization-induced microphase separation. **E.J. Lebron Perez**, W. Chan

Salon 3-4

Plenary 2

K. J. Noonan, K. A. Woznack, *Organizers*

5:00 244. Transition metal complexes for applications in photo-medicine and the production of solar fuels. **C. Turro**

Thursday Poster Session

162. Use of cyclic voltammetry for electrochemical characterization of electrode-coupled biofilms. **A. Castro**, A.R. de Andrade

163. Peruvian textile fibers: Sequential analysis and radiocarbon dating. **J. Williams**, R. Armitage

164. Biochemical analysis of quality indicators of three fish species sold at fish markets in Kuwait. **A. Anderson**

165. Comparison of excipients or impurities of brand-name and generic bupropion: Antidepressant and smoking cessation drug. **J. Sackey**, H. Holmes

166. Withdrawn

167. Collision-induced dissociation of protonated phenethylamine: A model study to aid illicit drug identification by tandem mass spectrometry. **A. Ihabi**, S.J. Lenze, J.G. Terhorst, T.A. Corcovilos, M.J. van Stipdonk

168. Developing a method to quantify cannabidiol (CBD) and Δ^9 -tetrahydrocannabinol (THC) in commercial CBD lotions. **K. Sonnie**, K.S. Wendling

169. Determining the caffeine content in decaffeinated coffee using HPLC. **H. Scott**, K.S. Wendling

- 170.** Determination of relative configuration of water-soluble molecules using anisotropic NMR. J. Cassani, **K.H. Schulz**, C.F. Tormena, R.R. Gil
- 171.** Exploring cytochrome c electrochemistry on peptide self-assembled monolayer modified gold electrodes. **M. Hargittai**, R.A. Clark, C. Weiland
- 172.** In pursuit of an Optical Ion Trap (OIT) mass analyzer. **L. Dugan**, F. Lanni, M.E. Bier
- 173.** Organophosphate esters (OPEs) in on-site wastewater treatment systems. **F. Li**, R. Smolinski, C.A. McDonough
- 174.** Withdrawn
- 175.** Dual emission system of fluorescent dye and folic acid carbon quantum dots for aerosol pH measurement. **A. Butzler**, E. Tackman, M. Freedman
- 176.** Effortless alkalinity analysis using AI and smartphone technology, no equipment needed, from freshwater to saltwater. **Z. Han**, Z. Zheng, A. Han, H. Zhang
- 177.** Uncovering PFAS bioaccumulation in seal livers: Insights from suspect screening and nontarget analysis using HPLC-IMS-QTOF-MS. **Y. Chen**, L. Mukhopadhyay, B.S. Crimmins, C.A. McDonough
- 178.** Cleaning the wastewaters of the fabric dyeing industry with TAML/peroxide. **D. Chakraborty**, X. Ma
- 179.** Clay-based amendments reduce PFAS bioavailability in soil: Dynamics of soil-pore water system. **R. Mukhopadhyay**, **D. Sanchez**, **C.A. McDonough**
- 180.** Exploring preliminary biocompatibility testing in coating development. **R.M. Postema**, C.B. Sims, M. fyfe, X. Tan, H. Wildschutte, J.C. Furgal
- 181.** Using environmental biofilm's corrosivity to monitor drainage sludge biofilm sanitization efficacy. **C. Gu**

- 182.** Development and characterization of engineered Rieske dioxygenases with non-native activity. **B. Rutkowski**, J. Froese
- 183.** Development and application of a novel assay system for the detection of the enzymatic dihydroxylation of aliphatic olefins. **E. Lautzenheiser**, E. Talley, J. Froese
- 184.** Engineering of Rieske dioxygenase variants with improved activity through remodeling of the substrate tunnel. **J. Stover**, B. Rutkowski, J. Froese
- 185.** Mineral composition of bioclasts from the Caribbean Sea by XRD studies with Rietvel refining. **A. Barbosa Lopez**, A. Guzman, Y. Calderon
- 186.** Interactions of DNA origami with silane based Self-Assembled Monolayers (SAMs). S. Kundu, **S. Moore**, A. Kumari, H. Liu
- 187.** Mechanochemical reaction cascade for ligand synthesis and the growth of metal-organic frameworks. **Z. Tegudeer**, W. Gao
- 188.** Synthesis, characterization, and bandgap modulation of Molybdenum disulfide via DNA origami functionalization and metal ion doping. **a. kumari**, H. Liu, M. Curtis, D. Estrada, a. de, M. Anantram
- 189.** Withdrawn
- 190.** Ligand-assisted synthesis of mixed halide perovskite nanoparticles: Impact on single-particle photo blinking, bleaching, and phase separation dynamics. **D. Athapaththu**, J. Chen
- 191.** Mechanochemical synthesis of square-octahedron metal-organic frameworks. **D. Gabel**, A. Jung, W. Gao
- 192.** Multimetallic post-synthetic modifications of copper selenide nanoparticles. **T. Gordon**, R. Sen, S. Millheim, J. Smith, J. Millstone
- 193.** Defect engineering in the mechanochemical synthesis of metal-organic frameworks. **T. Plant-collins**, W. Gao

- 194.** Hammick decarboxylation of pyrazinoic acid: First step for improved tuberculosis drugs. **U. Puthumana**, A. O'Neill, T. Elmore, J. Rohde, A. Rohde, D.W. Gray, M. Kanzelberger, J. Rohde, J.D. Evanseck
- 195.** Reaction rates of alkaline earth metal-methide cations. D. Wraga, J. Higdon, S.J. Lenze, **M. Van Stipdonk**, T.A. Corcovilos
- 196.** Infrared action spectra of bare and solvated uranyl nitrate and formate cations. **M. Van Stipdonk**, T.A. Corcovilos, S.J. Lenze, C. Bassil
- 197.** Ultrafast spectroscopy to connect microscopic and macroscopic phenomena of carbon dioxide in Ionic liquid-derived materials. **M. Liberatore**, S. Garrett-Roe
- 198.** Investigation of the reversible fluorescence quenching properties of copper nanoclusters. **T.R. Brewer**, S. Rayan, A. Ashgar
- 199.** Bond dissociation studies with SCF stability analysis against CASSCF. **L. Madureira**, T. Kowalewski
- 200.** Insights into chemical bonding using accurate quantum bond orders and populations models. **B. Zulueta**, J.A. Keith
- 201.** "Green" copper: An environmentally friendly alternative to metal ion spectroscopy in an introductory chemistry laboratory course. **M. Ritchey**
- 202.** Adaptation of the synthesis of 5,10,15,20 Tetraphenylporphyrin for the CEM microwave: Green chemistry in teaching and learning for orgo labs curriculum. **A.J. Nishbert**, N. Kashem, J. Korn-Heilner, D. Laviska, N. Khan
- 203.** Investigating the mechanochemical insertion of metals into polydentate ligands. **G. Ross**, J. Koval, j. dee, E.P. Zovinka
- 204.** Oxidation reactions by cobalt-superoxo complexes. **D.G. Ford**, Z. Aghaei, A.A. Opalade, T.A. Jackson
- 205.** Synthesis and characterization of a novel open ring macrocycle incorporating pyridine. **N. Ajayi**, C.J. Ziegler

- 206.** Stabilization and reactivity of neutral and cationic magnesium hydride complexes and clusters. **D. Bedillion**, A. Banks, J. Kelly, T. Montgomery, P. Lummis
- 207.** Cu-promoted β -*ipso*-hydroxylation of substituted benzophenones using a bidentate directing group and H₂O₂ as oxidant. **S. Goswami**, K. Gill, X. Yin, M. Swart, I. Garcia-Bosch
- 208.** Synthesis and deprotonation of pyridinyl diimidazolium salts to be used as Lewis base ligands in s-block metal catalyst formation. **A. Caputo**, D. Bedillion, A. Banks, P. Lummis
- 209.** Small molecule activation using organocalcium hydride complexes. **A.M. Banks**, D. Bedillion, P. Lummis
- 210.** 1,4-Diaminophthalazine Complexes of Re(CO)₃. **T. Jeaydi**, C.J. Ziegler
- 211.** Low-coordinate transition metal complexes using bulky indoline based ligands. **I. Minney**, N. Walsh, B. Dolinar
- 212.** Synthesis and characterization of isoindolines modified with secondary amines. **J. Bore**, C.J. Ziegler
- 213.** Synthesis of two-coordinate first row transition metal complexes. **A. Reynolds**, S. Noor, B. Dolinar, K. Fish
- 214.** Synthesis of group 13 and 14 Azadipyrromethene chelates for fluorescence imaging. **A. Funke**, P. Lummis, T. Montgomery, D. Chase, J. Wincko
- 215.** Withdrawn
- 216.** Synthesis of gadolinium-based nitroxide-bearing redox-sensitive MRI contrast agents. **R. Minney**, L. McFadden, B. Dolinar
- 217.** Synthesis and characterization of a manifold of (PP^XP)CoI₂ complexes. **M.C. Seith**, M.C. Fitzsimmons, C.M. Thomas
- 218.** Withdrawn

- 219.** Synthesizing and studying novel photosensitizers to be used in cancer research. **H. Roche**, T. Montgomery, P. Lummis, D. Chase
- 220.** Synthesis and characterization of clicked cubosomes-graphene oxide hybrid platform for synergistic cell targeting and drug delivery. **M.M. Hossain**
- 221.** Multiple sclerosis and SHMT1: Characterization of G-quadruplex and i-Motif secondary structures in the 5' UTR. **S. Hershey**, Z. Woon, C.J. Frye, D. Heisler, M. Mihailescu
- 222.** Chemistry of covalent aptamers. **J.T. Boette**, S. Albright, C. Rosenblum, A. Deiters
- 223.** Engineering exosomes through versatile oligonucleotide tethers. **C. Blum**, P. Campbell, S.R. Das
- 224.** Chemically acylated tRNAs are functional in zebrafish embryos. **C. Rosenblum**, A. Deiters
- 225.** Labyrinthine dynamics of the apical nonalooop of SARS-CoV-2 Delta s2m by MD and NMR. **J.A. Makowski**, A. Kensinger, M.A. Wirtz Martin, T. Matzel, A. Wacker, H.R. Jonker, H.J. Schwalbe, J.D. Evanseck
- 226.** Understanding mitochondrial G-quadruplex formation and their potential as therapeutic scaffolds. **S. Kavooosi**
- 227.** Electrophilic aptamers for covalent modification of proteins. **S. Albright**, M. Cacace, A. Deiters
- 228.** Polypurine Reverse Hoogsteen (PPRH)-based stabilization of G-quadruplexes in the MYC and KRAS promoters as novel therapeutic approaches for ovarian cancer. K. Elder, E. Ospina-Sanchez, **T. Brooks**
- 229.** Invasion of kRAS G-Quadruplex by γ PNA. Z. Yildiz, **C.T. Martin**, B.A. Armitage
- 230.** Best method to determine DNA G-quadruplex folding: The ^1H - ^{13}C HSQC NMR experiment. **J. Dickerhoff**, J. Jang, D. Yang

- 231.** Quantum-based sensing of microRNA biomarkers and cortisol using NV-center nanodiamonds. I. Rampersaud, **C. Fletcher**, M. Forren, C. Angell, W. Carson, A. Rampersaud
- 232.** Physiological recognition of the MYC G-quadruplex by berberine. **J. Dickerhoff**, N. Brundridge, S.A. Mcluckey, D. Yang
- 233.** Studying the effect of ionic strength on the adsorption kinetics of diffusive YOYO-1 dye to immobilized lambda DNA molecules. **S. Pandey**
- 234.** DDX5 helicase resolves G-quadruplex and transactivates MYC expression. G. Wu, Z. Xing, E.J. Tran, **D. Yang**
- 235.** Indenoisoquinolines bind the *MYC* G-quadruplex and downregulate MYC expression in cancer cells. **M. DeMoss**, J. Dickerhoff, M.S. Cushman, D. Yang
- 236.** Characterizing structure and function of the G-Quadruplex in the *BDNF* mRNA: A route towards translational regulation in adult hippocampal neurogenesis. **R. Palumbo**, M. Mihailescu
- 237.** Ni aptamer: DNA mimic of His-tag to recognize Ni-NTA. **R. Jahan**
- 238.** Characterization of TET3 5'-UTR G-quadruplex secondary structures with implications in multiple sclerosis. **E. Good**, R. Palumbo, M. Kasaju, M. Mihailescu
- 239.** Biophysical characterization of a G-quadruplex structure in the Sox2 mRNA 3' UTR and its interactions with FMRP: Implications for cancer. **L. Parsi**, C. Cunningham, M. Mihailescu
- 240.** Elucidating the role of G-quadruplex structure in mediating the interactions of miR-145-5p and FMRP with the 3'-UTR of *Oct4* mRNA. **M. Kasaju**, M. Mihailescu
- 241.** Effect of sequence variation on the degradation of bottlebrush copolymers. **E. Sun**, B. Elshazly, T. Meyer
- 242.** Probing neighboring chain effects on the degradation of bottlebrush copolymers. **B. Elshazly**, E. Sun, T. Meyer

243. Electric field induced crosslinking reactions in polymer electrolyte thin films.

P.M. Prem, D.D. Sarawate, K. Xu, E.J. Beckman, S.K. Fullerton-Shirey

Friday Oral Sessions

Heinz Room

Nucleic Acid Chemistry

B. A. Armitage, X. Tan, D. Yang, *Presiding*

8:30 245. Heterobivalent aptamers for targeting a single protein. **X. Tan**

8:55 246. Development of novel functional nucleic acid materials to elucidate cell receptor activity. S. Rhozkov, Y. Ng Cen, **P. Mallikaratchy**

9:20 247. Aptamer-assisted phage display: enhancing checkpoint inhibition with a peptide and an aptamer targeting distinct sites on a single PD-L1 protein. **S. Arya**, S. Thennakoon, C. Phuoc, A. Silwal, R. Jahan, R.M. Postema, H. Timilsina, A. Reynolds, X. Tan

9:40 248. Quantitative and multiplexed cellular imaging with fluorogenic RNA aptamers. R. Zheng, **M. You**

10:05 Intermission.

10:20 249. Covalent aptamers as a new class of protein-modifying reagents. S. Albright, J.T. Boette, C. Rosenblum, B. Payne, M. Dorogan, H. Gizenski, **A. Deiters**

10:45 250. Bifunctional acylating reagent for RNA 2'-OH: Functional control and conjugation. **K. Liu**, A.M. Kietrys

11:05 251. URIL-tagging: A new chemical method for intracellular tracking and delivery of RNA-protein complexes. **D. Bong**

11:30 252. Withdrawn

Salk Room

Diversity, Equity, Inclusion, and Respect (DEIR) in Chemistry

K. A. Woznack, *Organizer, Presiding*

9:00 Opening Remarks.

9:05 253. Exploratory polymer and cosmetic chemistry curriculum for high school students to build scientific skills and confidence. **C. Birch**, G. Sherwood, G. Silva

9:25 254. Light at the end of the COVID-19 pandemic tunnel: How Women Chemists Committee cultivates an inclusive environment that empowers women. **A.M. Balija**

9:45 255. ACS Committee on Committee's strategies for maximizing the volunteer experience on committees. **J.R. Berk**, B.M. Mathes, D. Krone

10:05 256. Advancing accessibility: Initiatives and achievements of the chemists with Disabilities Committee (CWD). **P. Basu**

10:25 Intermission.

10:40 257. Accessible Science Communication: Tips for inclusive science posters and data. **R. Jemison**

11:00 258. Allyship, advocacy, and ACS. **N.A. LaFranzo**

11:20 259. Walking the walk: Fostering a strong culture of diversity, equity and inclusion at Merck. **M. Giles**

11:40 Panel Discussion.

Ohio Room

General Organic Chemistry

K. J. Noonan, *Organizer, Presiding*

9:00 260. PK_a of water is 14.00, not 15.74: The story of Brønsted's intellectual journey and its misapplication today. **T.L. Neils**

9:20 261. Synthesis and crystal structures of 18-crown-6 stabilized potassium salts of dioxalatodiphenylstannate and oxalatotriphenylstannate. **J. Sun, M. Rahman, Y. Torres, T. Greaves, X. Song**

9:40 262. Adapting cyclic and non-cyclic N-oxides for use in cycloadditions. **T.D. Montgomery**

10:00 263. Withdrawn

10:20 Intermission.

10:40 264. Toward a universal toolbox for preparing clickable covalent probes for chemical biology-mediated drug discovery and development. **D.J. Lapinsky**

11:00 265. Exploring the therapeutic potential of novel organic molecules on HeLa cells: A journey of undergraduate research and peer mentoring. **A. Blank, E. Lyon, P. Doleno, C. Voges, M. Metro, T. Zabroski, C. DeCarlo, N. Vesey, C. Kriley**

11:20 266. Design and synthesis of natural product derivatives as antibacterials. **S. Bergmeier, S. Abdullai, O. Adegbite, M. Hawk, N. Priestley, J.H. Hoody, J. Alverson, E. Schwartz**

11:40 267. Surveying ligand-mediated helix 12 transitions within the human estrogen receptor α using bipartite tetracysteine display. **J.M. Holub**

Mellon Room

Machine Learning in Chemistry

G. Hutchison, O. Isaayev, D. Yaron, *Organizers, Presiding*

9:00 268. Machine learning study for remote controlled copper nanoparticle synthesis in a cloud lab. **S.R. Das**, R.M. Gonzalez

9:25 269. Active learning for computational drug discovery with applications in the CACHE Challenge #1. **S. Koby**, E. Gutkin, F. Gusev, F. Gentile, F. Ban, C. Narangoda, A. Cherkasov, O. Isayev, M.G. Kurnikova

9:45 270. Predicting hydrogen evolution reaction activity from photophysical properties of cyclometalated iridium(III) complexes. **Y. Wang**, E. Lopato, S. DiLuzio, L. Dong, C. Shao, D. Yaron, S. Bernhard, T. Kowalewski

10:05 271. AIMNet2-NSE: Tackling radical reactions with neural network potential. **B. Kalita**, R. Zubatyuk, O. Isayev

10:25 Intermission.

10:40 272. Combined quantum mechanics and machine learning models: QupKake for pKa prediction. **G. Hutchison**

11:05 273. Manifold kernelization to encode quantum information for machine learning. **T. Li**, V. Chelagamsetty, R. Jordan

11:25 274. Neural network architecture to predict turnover numbers (K_{cat}) for protein-substrate pairs with primary sequence information for proteins and structural information for substrates. **J. Zhai**, J. Wang

Frick Room

Rare Earths and Critical Materials

R. Lin, W. Zhang, *Presiding*

9:00 283. Withdrawn

9:20 284. On the intrinsic reactivity of the middle oxidation states of uranium: Reactions of $[U^{IV}F_2C_2H]^+$ and $[U^{III}F_2]^+$ with formic, acetic, propionic, and acrylic acids. **S.J. Lenze**, J.G. Terhorst, M.J. van Stipdonk, T.A. Corcovilos

9:40 285. Rare earth metals production by hydrogen processing. **M. Feng**

10:10 286. Novel functionalized adsorbers for solid-phase extraction of germanium, gallium and platinum group metals from complex aqueous solutions. **A. Karamalidis**, M. Patel, D. Zhang, P. Raj

10:40 Intermission.

10:50 287. Characterization inform sustainable recovery of critical minerals from fossil energy waste feedstocks. **M.Y. Stuckman**, C. Lopano, C. Hoffman, C. Chen, M. Barczok, J. Mackey

11:20 288. Correlations between the mineralogy and recovery behavior of Rare earth elements (REEs) in coal waste. B. Ji, **W. Zhang**

11:50 289. Portable fiber optic sensor for rare earth elements and other critical metals using photoluminescence methods. **S. Crawford**, J.P. Baltrus, K. Kim, W. Burgess, A. Adkisson, N. Diemler

Thompson Room

Geological Hydrogen

G. Liu, *Organizer, Presiding*

10:30 Opening Remarks.

10:40 290. U.S. Regional H2Hubs Program Overview/Update. **D. Fairclough**

11:25 291. Challenges in prospecting for geologic hydrogen. **E. Holubnyak**

Thompson Room

Geological Hydrogen

G. Liu, *Organizer, Presiding*

1:00 292. Advanced sensor technologies for H₂ pipeline and subsurface storage monitoring. **R. Wright**

1:30 293. Understanding the mechanisms of serpentinization reaction for hydrogen generation. **Y. Tang**, Y. Wen

2:00 294. Introduction to HyFIVE: A practical tool for hydrogen geological storage evaluation. **N. Lin**

2:30 Break.

2:45 295. Infrastructure of hydrogen pipeline transportation cost and economic models. **G. Liu**

3:15 296. Hydrogen industrial insights: Status and investment. **A. Mattson**

Frick Room

Rare Earths and Critical Materials

R. Lin, W. Zhang, *Presiding*

1:10 297. Benchtop assessment of critical metal uptake by hydrous manganese oxide under biotic and abiotic conditions. **T.J. Boothe-Lordon**, R.C. Capo, B.W. Stewart, T.A. Olds, C.E. Rosenfeld

1:30 298. Designing surface-modified biochar for sustainable recovery of critical minerals from acid mine drainage. **W. Tugume**, D. Talan, O. SANYAL, S. Grushecky, H. Amini

1:50 299. Rhamnolipids as a multifunctional platform for rare-earth element detection, extraction, and separations. **R.M. Stolley**, C. Boxley, B. Bruggeman

2:15 300. Rare earth elements (REEs) recovery and hydrochar production from hyperaccumulators. **S. Li**, W. Zhang

2:40 Intermission.

2:50 301. Impact of organic acids on the extraction of rare earth elements: Mechanisms and optimization. **P. Liu**, X. Wang, W. Zhang

3:15 302. Exploring the role of solution structure on the thermodynamics of rare-earth element chelation by polymers. **C. Gallagher**, M.D. Schulz

3:40 303. Separation and recovery of trace rare earth elements via controlled chemisorption and electrosorption processes. **W. Zhan**

4:00 304. Rare-earth element chelation thermodynamics using flexible and hydrophobic polymer pendant-groups. **C.C. Armstrong**, C. Gallagher, M.D. Schulz

Heinz Room

Nucleic Acid Chemistry

B. A. Armitage, X. Tan, D. Yang, *Presiding*

1:30 305. DNA G-quadruplex: Structures, functions, and drug targeting. **D. Yang**

1:55 306. G quadruplex structure within the 3'-untranslated region of hnRNPK affects its expression by controlling the accessibility of miR-1249-3p to its binding site. **M. Mihailescu**, C. Grey, M. Kasaju, B. Kelleher, L. Grimaldi

2:20 307. *BCL2* promoter DNA secondary structures serve as recognition sites for activation induced cytidine deaminase. **S. Kendrick**, M. McCrury

2:45 Intermission.

3:00 308. Development and application of oligonucleotide therapeutics to induce and stabilize G-quadruplex structures. **T. Brooks**

3:25 309. Shedding light on G-quadruplex sequences with remote controlled assays in a cloud lab. **S.R. Das**

3:50 310. γ PNAs as modulators of biomolecular condensates associated with Amyotrophic Lateral Sclerosis. **R. Sriram**, B.A. Armitage

Salk Room

Undergraduate Research

E. A. Baldauff, *Organizer, Presiding*

2:00 311. Performance of activated charcoal in gastrointestinal decontamination: A comparative study of common toxins. H.B. Wood, **S. Trickett**, J.T. Dosch, D. Cao, S.A. Sydlik

2:15 312. Directed evolution of cytochrome P450 for synthesis of pyrrole marine natural products. **H.N. Crusenberry**, T.L. Suyama, S. Guy, E. Shields, L. Garrett

2:30 313. Optimizing catalyst-semiconductor integration in hybrid photoelectrodes for light-driven CO₂ reduction. **M.A. Stewart**, G.P. Bein, M. Tanwar, x. jia, C. Dones Lassalle, R. Powers, Z. Fakhraai, N. Hazari, J.L. Dempsey

2:45 314. Modernizing and enhancing general and analytical chemistry courses through applied laboratory activities. **S. Yoon**, R.L. Myers

Salon 3-4

Plenary 3

K. J. Noonan, K. A. Woznick, *Organizers*

6:00 388. Spin and Symmetry: Investigating Magneto-Optical Properties of Transition Metal Complexes. **W. Transue**

Friday Poster Session

- 315.** Design and synthesis of δ -lactone derivatives: Exploring the therapeutic potential of a versatile scaffold. **S. ABDULLAI**, M. Hawk, S. Bergmeier, N. Priestley
- 316.** Potent and selective oxidatively labile ether-based prodrugs through late-stage boronate incorporation. **P. Geaneotes**, C.P. Hankinson, C. Afeke, A. Deiters, P.E. Floreancig
- 317.** Green chemistry principles in process development. **S.D. McCann**
- 318.** Synthesis of aza-heterobicyclic small molecule degraders of the androgen receptor. **T.J. Casad**, R. Cole, W. Chen, A. Redhair, J.B. Nelson, Z. Wang, P. Wipf
- 319.** Design, synthesis, and evaluation of novel phenethylamine photoaffinity labeling probes. **F.E. Latherow**, C.J. Widman, D. Walther, M.T. Akere, A.N. Liddy, A.S. Wisner, I.E. Kaba, T. Nwaka, G.P. Tannish, L.E. Kountz, G.K. Boparai, S.P. Dressel, F.S. Hall, F.E. Williams, M.H. Baumann, I.T. Schiefer
- 320.** [3+2] cycloadditions of tertiary amine *N*-oxides to generate novel *N*-heterocycles. **N.A. Frankos**, T. Montgomery
- 321.** LDA aggregates in [3+2] cycloadditions of azomethine ylide with styrene: Third dimension of the Pople Diagram. **E. Chartier**, A. Cocolas, T. Montgomery, J.D. Evanseck
- 322.** Synthesis and optimization of [3+2] cycloaddition precursors for *N*-heterocycle formation. **M.M. Glista**, N.A. Frankos, A. Lane, A.H. Cocolas, T. Montgomery
- 323.** Iridium-catalyzed heterocycle formation using alkyne-tethered esters and imides. **J. Corcoran**
- 324.** Withdrawn

- 325.** Conditional control of benzylguanine binding to the self-labeling SNAPtag protein. **I. Demyan**, S. Caldwell, A. Parikh, G. Falcone, J. Lohmueller, A. Deiters
- 326.** Biocatalytic aza-Michael addition of aromatic amines to enone using α -amylase in water. **S. DUTT**
- 327.** Synthesis of functionalized reactants for the preparation of a more soluble benzylammonium ion. **V. Finizio**, P.A. Bonvallet
- 328.** Expanding precursory oxidative steps of *N*-heterocycle synthesis through a novel [3+2] cycloaddition. **J. Graber**, N.A. Frankos, A. Lane, A.H. Cocolas, T. Montgomery
- 329.** Towards an alkylated porphyrin-PYBOX: Advances in porphyrin solubility through the addition of dodecyl groups. **G. Hayes**, P.A. Bonvallet
- 330.** Total synthesis and structural determination of Neaumycin B: Studies of the C-34 stereochemistry. **A. Healy**, N. Cinti, M. Van Engen, P.E. Floreancig
- 331.** Synthesis and photochemical evaluation of new photoswitchable amino acids. **M. Hill**, O. Shade, A. Deiters
- 332.** Advances in the synthetic methods of porphyrin-PYBOX macromolecules. **M. Johnson**, P.A. Bonvallet
- 333.** Exploring new routes to chrysochlorin D: A potential avenue toward effective chemotherapy. **T.N. Kiss**, A. Lane, A. Cocolas, T. Montgomery
- 334.** Design of a bifunctionalized boron allyloxy-caged linker and demonstration of hydrogen peroxide-mediated cargo release. **B. Klootwyk**, G. Fleury, P.E. Floreancig
- 335.** Optimization and synthesis of 7-Azanorbornanes using tertiary amine *n*-oxides and substituted alkenes. **A. Lane**, A. Cocolas, T. Montgomery
- 336.** Utilization of density functional theory to optimize the synthesis of *N*-heterocycles. **K.M. Luca**, N.A. Frankos, N. Ozimek, J.P. Moerdyk, T. Montgomery

- 337.** Investigation of cationic fluorenylmethoxycarbonyl phenylalanine hydrogels with different C-terminus linkers. **T.K. Luu**
- 338.** Directed evolution of Cytochrome P450 to synthesize natural products. **R. Mittendorf**, S. Guy, T. Dohn, H.J. Fletcher, T.L. Suyama
- 339.** Improving the diastereoselective synthesis of spiro- and fused-cyclobutane bearing 4-aminotetrahydroquinolines: Applications towards Kv7.2/7.3 agonists for the treatment of tinnitus. **M. Morton**, C. Hill, P. Wipf
- 340.** Synthesizing a novel carbene: Offering new capabilities in transition metal-free catalysis. **N. Ozimek**, **J. Hampton**, K.M. Luca, T. Montgomery, P. Lummis, J.P. Moerdyk
- 341.** Asymmetric approach to novel small molecule androgen receptor antagonist development. **C. Pratt**, P. Wipf, J.B. Nelson, R. Cole, W. Chen, Z. Wang
- 342.** Development of small molecule drugs at Merck: From hit identification to development candidate and scale-up of a novel STING agonist. **R.J. Rahimoff**
- 343.** Alkyl halides via visible light mediated dehalogenation. **M. Rathnayake**, J.D. Weaver
- 344.** Napabucasin analogues with increased bioavailability and efficacy in fibrolamellar hepatocellular carcinoma. **S. Rawat**, J. Alderman, L. Hartshorn, C. Villasenor, P. Baeza, B. Lyons, J. Brazil
- 345.** Oxocarbenium ion 5-membered ring conformational energies and geometries by DFT and MP2: Foundation for predicting acetal substitution diastereomeric ratios. **E. Rodo**, J.A. Makowski, J.D. Evanseck
- 346.** Synthesis, *in-silico* studies, and anticancer activity of curcumin derivatives. **A.C. Bamigboye**, T. Salam, H. Abbo
- 347.** Synthesis and vinyl-addition polymerization of short-tethered cationic norbornene monomers. **K.H. Schulz**, R.R. Gil, K.J. Noonan

348. Withdrawn

349. Developing novel azadipyrromethene derivatives for diagnostic medicine. **L.J. Sweeney**, T. Montgomery

350. Transition metal mimetic π -activation by Cationic bismuth(III) catalysts for allylic C–H functionalization of olefins using C=O and C=N electrophiles. **R. Wang**

351. Umpolung Nicholas reaction analogue for C–H propargylic etherification. **Y. Xia**

352. Career pathways in chemistry: Balancing the transition into new leadership roles. **L.J. Nogaj**

353. Evaluation of anticancer effects by different fragments of amyloid- β on non-small cell lung cancer cells. **I. Seidu, H. Evans, D. Heyl-Clegg**

354. Chemistry-based assembly and control of antibody-directed enzyme prodrug therapy. **M. Charette, N. Paul**, G. Falcone, A. Deiters

355. Analytical research & development at Merck: Leveraging diverse expertise to be partners in problem solving. **S. Chugh**

356. Withdrawn

357. Chemical tool to synthesize and investigate glutathionylated proteins. **D. Oppong**

358. Case study of Korean-style steam education in teacher training colleges (2): visualizing the shape of a typhoon with changes in atmospheric pressure. **K. Young Tae**

359. Case study of Korean-style STEAM Education in Teacher Training College (1): Is it desirable to open classroom windows for ventilation even when the concentration of fine dust in the air is high? -. **K. Young Tae**

- 360.** Experimental validation for machine learning model-calculated ring strain by ring opening metathesis polymerization. **J. Vinskus**, Z. Liu, K.J. Noonan, O. Isayev
- 361.** Effective quest into bounded chemical space: A case study of aromatic amines/imines. **Y. Wang**, **R. Sarma**, C. Shao, C. Yang, I. Garcia-Bosch
- 362.** Exploring a novel immune modulation approach for monomeric Interferon Gamma (IFN γ) design. **A. Guo-Yue**
- 363.** Greener solutions for synthesizing nanoparticles and quantum dots. **T. Cree**, A.M. Smith-Diemler
- 364.** Identification of host substrates for the secreted internalin proteins from *Listeria*. **M. Lyons**, D. Heisler
- 365.** R.O.C.K. program: Bringing hands-on science into local schools. **M. Hogue**, A.M. Smith-Diemler, S.E. Evans
- 366.** ATP: An alternate role of an energy currency. **T. Erben**, J.A. Makowski, A. Kensinger, J.D. Evanseck, D.W. Seybert
- 367.** Co²⁺ doped Ag-TiO₂ hybrid nanocrystal photocatalysis: Applications in renewable energy. **Q.D. Williams**
- 368.** Screening imidazole derivatives for their antibacterial activity against foodborne pathogens. **T.G. Newman**, N.A. Frankos, A. Lane, T. Montgomery, D. Heisler
- 369.** Mapping the binding site of a novel paroxetine analog on the serotonin transporter with crosslinking and mass spectrometry. **E. Stahovich**, S. Aranibar-Chang, W. Lowther, L. Bohrer, D. Lapinsky, M. Cascio
- 370.** Site-directed mutagenesis of alpha-synuclein. **K. Walker**, E. Parker, J.L. Sarver
- 371.** Photochemical studies of Anticancer Ruthenium-Platinum bimetallic complexes adsorbed on Montmorillonite. **P. Bradley**, N. Conroy, A. Maicaneanu, A. Jain

- 372.** PROFIND: Innovative computational techniques for PROTAC synthesis. **A. Goel**, G. Sharma
- 373.** Pre and post-processing effects of protein structure in dynamic thermosets. **Y. Foong**, S. Surprenant, W. Chan
- 374.** Applying CRISPR-Cas12 as a signal enhancer for PFAS detection. **B. Platt**, E. Ajibode, K. Yehl
- 375.** Studying the behavior of holmium and its interactions with a multi-dentate ligand to model analogous behavior in siderophore containing bacteria. **K. Frankowski**
- 376.** From pepper to particle: A green synthesis of pseudospherical gold nanoparticles. **A.R. Seese**, A.M. Smith-Diemler
- 377.** Synthesizing strong bonds between students and faculty at Saint Francis University. **A.R. Seese**, M. Hogue, G. Ross, T. Cree, M. Wheeler, A. Ochs, A.M. Smith-Diemler
- 378.** Synthesis of fluorescent warheads for aptamer-mediated multiplex labeling. **B. Payne**, J.T. Boette, S. Albright, A. Deiters
- 379.** Prevention of lipid oxidative damage in model membranes by antioxidant supplementation. E. Hardwick, M. Kunes, A. Niemesh, K. Winey, **Z. Graber**
- 380.** Biochemical characterization of Galactokinase 1. **M. Stewart**, A. Cooper-Morgan
- 381.** Characterization of honey in Northwest Ohio: An investigation of its contents. **C. Colahan**, **K. Grow**, **E. Keto**, **M. Sage**, B.G. Vanness
- 382.** Photoelectron transfer in halogen-bonded complexes of bromosubstituted electrophiles with halide anions. **M.C. Hardin**, A. Burnell, S.V. Rosokha
- 383.** Characterizing the effects of hydrogen bonding in glycylglycine hydrochloride and glycine hydrochloride systems. **M. Joyce**, E. Chartier, R. Iulucci, J.D. Evanseck

- 384.** Characterization of CuBDC surMOF film formation via Infrared-reflectance absorbance spectroscopy. **K.E. Coffin, S. Delozier, D. Maglich,** K. Euston, M.E. Anderson, C.M. Mauck
- 385.** Assessment of McKean County drink water preferences. **H. Gordon, O. Femi-Oloye, M. Odorisio, O. Francestscu, R. Myers, F.F. Oloye**
- 386.** Heidelberg University's ACS chemistry club trips. M. Sage, **S. Grosse,** N. Beres, B.G. Vanness, B.D. Smith, C. Colahan
- 387.** Exploring Acid Mine Drainage (AMD) as a civic engagement project. **M. Swaim,** E.P. Zovinka

Saturday Oral Sessions

Heinz Room

Undergraduate Research

E. A. Baldauff, *Organizer, Presiding*

8:30 389. DNA origami nanoimprinting biologically compatible polymers. **D.A. Santia**, A. Kumari, H. Liu

8:45 390. Hofmeister effect on the pKa of small molecules. **A.J. Mosier**, F.F. Oloye, R.L. Myers

9:00 391. Bottlebrush polymer synthesis using a 5-norbornene-2,3-carboxylic acid anchor group. **B.R. Price**, B. Elshazly, T.Y. Meyer

9:15 392. Withdrawn

Heinz Room

Undergraduate Research

E. A. Baldauff, *Organizer, Presiding*

2:00 393. My experience at Brookhaven National lab's nuclear Chemistry Summer School. **J. Samol**

2:15 394. Biodegradable and renewable protein-based elastomers. **I. Cui**, W. Chan

2:30 395. Synthesizing protein-copolymers via grafting-from photopolymerization. W. Chan, **E. David**

2:45 396. Anthraquinone motifs as ligands and host molecule: Synthesis, complexation and characterization. **A. Jezorski**, K. Mariappan

3:00 397. Self-healing polyurethane derived from thermally reversible network blocking-deblocking. **D. Johnson**, H. Sodano

3:15 398. Exploration of Deep Eutectic Solvents and Nickel-plated graphite felt electrodes in supercapacitors. **D. Alarcon**, D. Soriano, F.F. Oloye, R.L. Myers

3:30 399. Probing the role of acidification on activity of plantain peel-derived activated carbon for removal of green dye from wastewater. **H. Gordon**, R. Myers, **F.F. Oloye**

3:45 400. Wave-particle duality of the Kamehameha a creative approach to understanding quantum mechanics. **A. Barbosa Lopez**, L. Ayala Bertel, R. Hernandez

Workshops and Activities

Wednesday

Industry Workshops

9 AM - 12 PM

“A Coating Primer with PPG”: Have you ever wondered how coatings protect and beautify objects that you interact with every day? Join PPG to learn more about the exciting world of paints & coatings at our Coatings Fundamentals Design Thinking Workshop! We will explore the chemistry and physics behind coatings and learn about different types of coatings, their properties, and characterization techniques. Throughout the session, participants will have the opportunity to apply design thinking principles to solve real-world coatings problems to facilitate active learning and practical application of the concepts covered.

9 AM - 10:30 AM

“Coal and Waste Coal to Advanced Material Products: Carbon Foams, Graphite Foams, and Coal-Plastic Composites with CONSOL Energy”: CONSOL Innovations is a subsidiary of CONSOL Energy focused on developing and commercializing new advanced carbon materials and products that can be derived from coal or waste coal feedstocks. Waste coal includes the fine and ultra fine particulates that are produced during the coal mining and preparation process. Utilization of these waste fines prevents their disposal in surface impoundments, and may eventually lead to remediation of impoundment sites and production of valuable products. This short course will provide an overview of our coal-based vitreous carbon and pitch-based graphite foams and their applications in the aerospace/defense, battery, and building materials industries, as well as our work developing coal-plastic composites from coal and waste coal for building materials. We will also discuss our strong relationships with University partners and small businesses that promote rapid research and development efforts and commercialization of new technologies.

Networking Luncheon

12 PM - 1 PM

This luncheon serves as an opportunity to network with others, create dialogue, and build community, where all attendees are warmly welcomed. (\$25 per person / \$10 per student)

Brewery Workshop

1 PM - 3:30 PM

Join us as Abstract Realm Brewing Company provides a tasting and workshop on the art and science of brewing. Register for \$30 per person with your CERM registration. As a founding member of a financial planning firm and hobby homebrewer, Abstract Realm principal owner Jason Short had seen his share of successful (and unsuccessful) small business ventures from others. Driven by fond memories of joining his grandfather at the local bar and seeing the way it provided a social outlet for the community, Jason decided that the Hazelwood Brewhouse project provided the perfect opportunity for a place of his own. Head brewer and co-owner Chris, who has spent the last decade making his rounds brewing at a handful of Pittsburgh Breweries including Brew Gentlemen and Aurochs, shares Jason's vision of Abstract Realm being a place where people of all walks of life can share a beer, a story, and continue to build on the diversity of Pittsburgh. This shared vision laid the base for the mission statement as well as the name Abstract Realm. For Jason and Chris the use of "abstract" represents the concept of transcending boundaries or having "no limits" through the use of innovative brewing techniques, while at the same time inviting everyone into a realm of creativity, inclusivity, and community.

Committee on International Activities Cocktail Hour

4 PM - 5 PM

Join us before the first Plenary Lecture to network and celebrate the start of CERM 2024. The cocktail hour is sponsored by the ACS Committee on International Activities (AIC).

ACS Governance Reception

6 PM - 7:30 PM

Join us in an evening of networking and fun. We will be joined by three members of the ACS Board of Directors: Wayne Jones, Lisa Balbes, and Natalie LaFranzo.

Glassblowing Demonstration at the Pittsburgh Glass Center

8:30 PM - 9:30 PM

Join us on a tour and demonstration on the art and science of glassblowing. Register for \$20 per person with your CERM registration. Attend an exciting live narrated glassblowing demonstration and watch expert artists create amazing glass art in our state-of-the-art studios. Learn about Pittsburgh's lesser-known but incredibly rich glassmaking history and take a guided tour of our contemporary glass art exhibition in the Hodge Gallery. This option does not include a hands-on experience. Established in 2001, Pittsburgh Glass Center (PGC) is a nonprofit, public-access education center; an art gallery; a state-of-the-art glass studio; a community builder; and a hub for innovation and creativity. Anyone can take classes, explore the contemporary glass gallery, and watch the live hot glass demonstrations. World-renowned glass artists come here to both create and teach. The Pittsburgh Glass Center is 20-25 minutes from CERM 2024.

Thursday

Exposition

Check out the exhibitors at the CERM 2024 Expo in the Ballroom. The Expo will be open from Thursday, November 7 at 9 AM to Friday, November 8 at 4:30 PM.

Industry Workshops

9 AM - 12 PM

“Advanced Tube Bending Workshop with Swagelok”: More connections equal more potential leaks. We'll give you the foundational knowledge needed to introduce bent tubing to your system to eliminate joints and leak points inherent

in traditional welded-pipe systems. Learn how to: properly cut and deburr tubing, understand various marks used in tube bending, bend tubing with the correct bend angle made in the correct location, identify five potential bend defects, and expertly assemble a box comprised of various lengths of tubing bent according to requirements. Our certified technical trainer, Mike Gagel, will ensure that you learn how to properly and safely bend tubing to get optimum value from your Swagelok componentry investment. Swagelok® Technical Training classes deliver an unparalleled depth of timely and leading-edge content – supplemented with actual hands-on practice – to help significantly reduce your installation errors, excessive maintenance downtime, and overall operating expenses! Graduates receive a genuine Swagelok Certificate of Completion for Install/Inspect and Bending! "We'll help you understand exactly what you're trying to make before any tube is bent. We'll then show you how to mark the tube prior to use of a hand bender to accurately make the bends - in minimal time and without scrap"

1 PM - 4 PM

“Science-based Artificial Intelligence/Machine Learning Workshop with National Energy Technology Laboratory”: The Science-based Artificial Intelligence and Machine Learning Institute (SAMI) leverages science-based models, artificial intelligence, and machine learning (AI/ML) methods, data analytics, and high-performance computing to accelerate applied technology development for clean, efficient, and affordable energy production and utilization. These advances empower NETL to push the frontiers of AI technology and create next generation architectures, tools, and approaches, expand partnerships to advance the development and adoption of AI, and foster AI workforce development. The Institute combines the expertise of NETL’s energy computational scientists, data scientists, and subject matter experts with strategic partners to enable AI-driven solutions and support to applied energy science, environmental and social justice, and other strategic objectives within DOE’s and NETL's missions. Outline of the Workshop: NETL and SAMI, Energy Data eXchange (EDX), Internships/Fellowships/Recruitment at NETL, AI/ML in Materials Science

Environmental Group Luncheon

12 PM - 1:30 PM

Join the Pittsburgh Section's Environmental Group for a Luncheon with Keynote Speaker, Jenalle Brewer. Jenalle will give a global and regional view of the PFAS landscape, and the ways in which the EPA and companies like Calgon Carbon are tackling these emerging contaminants.

Recent findings by the U.S. Geological Survey reveal that at least 45% of the nation's tap water is estimated to contain one or more types of per- and polyfluorinated alkyl substances, or PFAS, a group of man-made chemicals widely known as "forever chemicals" due to their persistence in the environment. In response, the Environmental Protection Agency (EPA) has established national limits for six specific types of PFAS in drinking water, highlighting the critical need for effective solutions.

Calgon Carbon Corporation, a Pittsburgh-based global leader with over 80 years of experience in activated carbon manufacturing and technology, is at the forefront of addressing this challenge. By providing advanced activated carbon products and services, Calgon Carbon plays a critical role in removing PFAS from both drinking water and wastewater, offering a powerful, locally developed strategic solution to this global environmental threat.

Jenalle Brewer, Senior Vice President, Drinking Water Solutions & Global Business Development will give a global and regional view of the PFAS landscape, and the ways in which the EPA and companies like Calgon Carbon are tackling these persistent contaminants.

Add the Environmental Group Luncheon to your CERM 2024 registration via the conference registration page! The cost is \$35 per general attendee or \$10 per student attendee.

Awards Dinner

6 PM - 8 PM

Join us at a dinner and awards ceremony that will celebrate the achievements of ACS members.

Friday

Exposition

Check out the exhibitors at the CERM 2024 Expo in the Ballroom. The Expo will be open from Thursday, November 7 at 9 AM to Friday, November 8 at 4:30 PM.

ACS Career Workshop

9 AM - 12 PM

“Finding Yourself: Identifying a Career that Matches your Strengths and Values”:

This course provides self-assessment tools to identify career values and strengths. Participants will compare and contrast the four sectors of chemistry employment to determine which sector best aligns with their values and strengths. This data will then be used to create a targeted job search strategy. Key topics include how to: Identify and describe your values and strengths in terms of employability, compare and contrast job market outlook and skills in industry, academia, government, and self-employment sectors, understand the purposes of networking, and apply questioning strategies to engage in effective networking.

Women Chemists Committee Luncheon

12 PM - 1 PM

Join the Pittsburgh Section’s Women Chemists Committee for a Luncheon with Keynote Speaker, Natalie LaFranzo, an ACS Director-at-Large. Natalie will speak on the topic of “non-traditional” careers in chemistry. All are welcome to attend.

Natalie A. LaFranzo is the Vice President of Strategy at LINUS. She earned her Bachelor of Science degree in chemistry from Bradley University in 2007 and her Ph.D. in chemistry from Washington University in St. Louis in 2013. She has held numerous commercial roles in biotech, with a focus on genomics and precision medicine. She served as the Director of Marketing Communications at Personalis and was Vice President of Market Development at Cofactor Genomics, an RNA diagnostics company. She has been a member of the American Chemical Society since 2007, where is she has served at the Local Section level, Divisional Level, Regional Level, National and International Levels. She has also served on several

ACS committees including the Council Policy Committee, the Committee on Budget and Finance, and as Chair of the Younger Chemists Committee. Her interests include creating inclusive environments, team building, business development and corporate collaborations, start-up/small business growth, marketing, scientific writing, collaborations, and leadership development. Add the WCC Luncheon to your CERM 2024 registration via the conference registration page! The cost is \$35 per general attendee or \$10 per student attendee.

ACS Resume Review Workshop

1 PM - 3 PM

One on one interviews scheduled onsite for review of individual resumes.

SMID-DEIR Workshop

1 PM - 5 PM

“The Science of Managing Inclusive and Diverse Teams”: The Science of Managing Inclusive and Diverse Teams provides evidence-based guidance and structure to chemistry professionals so they can create and maintain a diverse, equitable, inclusive and respectful workplace. After this workshop, participants will be able to:

- Become familiar with common identity types that scientific and census protocols use to analyze groups of people.
- Apply Tuckman’s “Stages of Team Development” model to past, current and future teams.
- Differentiate between various social identity models as it pertains to the individual.
- Practice and apply an empathy model to remove barriers to professional success based on intersectional social identity models.

Undergraduate Networking Reception

4:30 PM - 6 PM

This reception serves as an opportunity to network with others, create dialogue, and build community, where all attendees are warmly welcomed and encouraged to participate.

Saturday

Graduate School Fair

9:30 AM - 11 AM

Meet representatives from a range of graduate programs in our central region and beyond.

(1) Duquesne University Department of Chemistry, (2) Florida State University Department of Chemistry, (3) Ohio University Departments of Chemistry and Chemical Engineering, (4) West Virginia University Department of Chemistry, (5) University of Cincinnati Department of Chemistry, (6) University of Pittsburgh Department of Chemistry, (7) University of Pittsburgh Molecular Biophysics and Structural Biology Program

Additionally, speak with current graduate students from the region about how to apply to graduate school and what it is like!

PennWest University Workshop

9:30 AM - 11 AM

“Better Together: The Development of Cross-Disciplinary Faculty Learning Communities in Higher Education”: Our institution was recently awarded an NSF IUSE grant to implement a cross-disciplinary learning community. A learning community has a facilitator, resembles a focus group, and allows instructors to have conversations centered on instruction and student learning. In this workshop, we will explain how we implemented our learning community, our thoughts as participants, preliminary findings, and how others could implement a learning community at their institutions. Preliminary findings include: (a) every instructor (n=20) at our institution is participating, but attendance was a challenge at times, (b) instructors experimented with different instructional approaches, (c)

instructors believed strategies impacted student learning, (d) instructors stated that learning communities differed from their expectations and provided a much-needed forum to discuss shared challenges, (e) facilitators stated some tension between the intended focus and the free-form structure of the learning community; and (e) the first learning community cohort has independently sustained itself apart from the original project.

Applying to Professional Schools Workshop

11 AM - 12 PM

Come hear from a variety of healthcare workers their journeys from undergraduate studies to practicing in medical careers!

Pre-Professional Career Panel

1 PM - 2 PM

What can you do with a degree in chemistry or a related field? Come hear from a variety of different professionals discuss their career pathways and day-to-day work.