RMRM 2025

THURSDAY MORNING

General Materials Chemistry

Alvarado Salon G

Cosponsored by PHYS
S. Bobbitt, *Organizer, Presiding*

8:00 Introductory remarks.

8:05 001. Harnessing cocktail effects: A computationally guided approach for optimizing catalytic activity in high-entropy metal–organic frameworks (HEMOFs). **J. Geary**, D.J. Vogel, P.G. Kotula, M. Meyerson, C.E. McKeown, M. Steinberg, D.F. Sava Gallis

8:30 002. Developing a 2D platform for dynamic covalent MOFs. **D. Fairchild**, L. Appelhans

8:55 003. Heterometal doped aluminum oxide for remediation of per- and polyfluoroalkyl substances (PFAS). **M. Shohel**, N. Bays, S. Kruse, A.A. Chacon, N. Barrett, R.D. Davis

9:20 Break.

9:35 004. Tuning the structure of Thienoisoindigo (TIG) copolymers to afford bright near-infrared emission for bioimaging through aggregation-enhanced emission. **R. Posey**, C.B. Cashman, N. Gill, J. Tropp

10:00 005. Impact of chemical disorder on electronic properties of composition-dependent refractory alloys. **S.T. Bijjala**, P. Kumar, S.R. Atlas

10:25 Break.

10:40 006. Rapid fabrication of grayscale lithography masks via annealed resin Engineering. **T. Creason**, B. Kaehr, B. Burckel

11:05 007. Stabilizing zinc porphyrin supramolecular polymers to control structure–function relationships in organic solvents. **I. Tsironi**, E. Orcutt, J. Maleszka, E. Grumstrup, J. Olivier

Materials for Electrochemical Energy Storage and Conversion

Alvarado Salon A

Cosponsored by ENFL
D. Chen, *Organizer, Presiding*

8:00 Introductory remarks.

8:05 008. Rechargeable Al-CO_2 battery enabled by a homogeneous redox mediator. **S. Wei**

8:35 009. Design principles from the multi-electron redox reactions of conversion cathode materials. **E. Mozur**

9:05 010. Evolution of site selectivity in electrochemical CO_2 reduction on Cu. **J. Yan**, Y. Kim, J. Ager

9:25 Break.

9:40 011. Manganese-based disordered cathode materials for lithium-ion batteries. **J. Ahn**

10:10 012. Small-angle neutron scattering characterization of dispersions of short and long side chain ionomers: toward improving proton exchange membrane fuel cells. **R.P. Hjelm**, J. Klein, M.E. Hawley, C.F. Welch, A. Sokolova, S. Yim, Y. Kim

10:30 013. Electron localization in cation-disordered rocksalt cathode materials. **A. Outka**, H. Ho, Y. Wang, B. Raji-Adefila, W. Kuo, J. Watt, D. Chen

10:50 Break.

11:00 014. Energy-saving seawater splitting coupling sulfion recycling over a CuCo layered double hydroxide electrode. **Y. Fei**, Q. Mao, X. Liu, W. Li, M. Zhou

11:20 015. Tunable bifunctional nickel sulfoselenides for oxygen electrocatalysts in Zn-air batteries. **J. Espano**, J. Pillars, T.N. Lambert, B.R. Wygant

11:40 016. Probing the health status of electrolyte and interphase in battery cells via fiber-optics-based autofluorescence sensing system. **D. Chen**, Y. Wang, B. Raji-Adefila

Cement, Clays, and General Geochemistry

Alvarado Salon F

Cosponsored by GEOC
J. A. Greathouse, M. Mills, *Organizers, Presiding*

9:00 017. Accurate force fields for atomistic simulations of oxides, hydroxides, multivalent ions, and organic hybrid materials up to the micrometer scale. K. Kanhaiya, R. Mishra, P. in't Veld, I. Nikiforov, Y. Choi, C. Zhu, W. Im, E. Tadmor, **H. Heinz**

9:30 018. Beyond force field mixing rules to model silica-water interfaces. **T. Jayawardena**, S.M. Godahewa, W.H. Thompson, J.A. Greathouse

10:00 Break.

10:10 019. THAMES: Relating structural evolution of porous multiphase media to their environmental conditions through 3D microstructure simulations. **J.W. Bullard**, F. Nita

10:30 020. Exploring spontaneous oxidation chemistry at the air-water interface of microdroplets. **P.R. Tumminello**, N. Bays, D. Schafer, L. Sheps, J.A. Echternach, C.J. Kliewer, R.D. Davis

10:50 021. In-situ observation of mafic/ultramafic rock reactions with supercritical CO_2 using neutron reflectometry. **C.W. Neil**, E. Watkins, C. Neal, C. Keeter, C. Halbert, J. Browning, H. Viswanathan

Medical Science Chemistry

Alvarado Salon C

Cosponsored by MEDI
R. Polt, *Organizer, Presiding*

9:00 Introductory remarks.

9:05 022. Glycopeptide drugs from endogenous neuropeptides. T.E. Smith, M. Cai, M. Heien, T. Falk, R. Khober, N.J. Christie, F.A. Al-Obeidi, F. Nugent, **R. Polt**

9:30 023. Synthesis and alpha-glucosidase inhibition potencies of paprazine derivatives as potential diabetes medications. **M.A. Christiansen**, W. Hatch, B.J. Williams, T.L. Carter, S.I. Hanifin, K. Zager, J. Scepaniak, B. Holmes, B. Floyd, S. Bryner, S. Nelson, E. Sharp, A. Lester

9:55 Break.

10:10 024. Design, synthesis, and study of opioid cyclic tetrapeptides. **M.J. Ferracane**

10:35 025. Toxicology review papers: An editorial perspective based on 50 years of publishing. **R.O. McClellan**

11:00 026. Vanadium drug loaded carbon nanodots as novel therapeutic materials for intertumoral administration in the treatment of glioblastoma. **A. Miller**, E.D. Dukhovskaya, B. Yett, A. Banerjee, D.C. Crans

Molten Salt Chemistry

Alvarado Salon DE

Cosponsored by NUCL
M. Christian, D. Eralie, *Organizers, Presiding*

9:00 Introductory Remarks.

9:05 027. Chromium solution in molten uranium-sodium chloride salts investigated by ab initio molecular dynamics simulations. **A. Andersson**

9:25 028. Synthesis of UCl_3 and solid-state NMR spectroscopy studies. **S.R. Lee**

9:45 029. Updates on neutron investigations of UCl_3-bearing molten salts. **M.J. Monreal**, S. Vogel, A. Andersson, H.K. Patenaude, J.C. Neuefeind

10:05 Break.

10:25 030. Measuring the enthalpy of mixing of molten NaCl-UCl_3 salt by high temperature drop calorimetry. **B.E. Merrill**, H.K. Patenaude, D. Eralie, J. Chamberlain, N. Rood, S.S. Parker, H. Boukhalfa, X. Guo, M.J. Monreal, H. Xu

10:45 031. Calorimetric measurements of actinide-bearing molten salt systems. **H.K. Patenaude**, S.S. Parker, M.J. Monreal

11:05 032. Novel approaches to measure the viscosity and density of molten salts. **D. Eralie**, H.K. Patenaude, S. Peyres, C. Hatfield, A. Long, S.S. Parker, M.J. Monreal, M. Jackson

11:25 033. MELCOR solid particle transport modeling in molten salts. **M. Christian**, D. Luxat

Sensor Technologies

Alvarado Salon B

Cosponsored by PHYS
S. Percival, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 034. Design of a modular diazaborine-based ratiometric probe for detection of peroxynitrite in biological systems. **M. Melville**, A. Mailand, D. Domaille

9:30 035. Biomimetic surface enhanced Raman scattering sensor for in-situ analyte detection in biofluids. **G.W. Greene**, M. Han, P. Stoddart

9:55 036. *Operando* investigation of transduction and reception functions of Ga_2O_3 chemirisistive H_2 sensors using a Spectro-Electrochemical Set-up. **K. Valeti**, W.A. Callahan, K. RAFIQ, D. Klotz, A. Zakutayev, R. O'Hayre, A. Staerz

10:20 Break.

10:35 037. Ohm-Sweet-Ohm: Intradermally implantable, conductive tattoo ink for human–computer interaction and bioelectronic integration. **J. Coffie**, M. skandarajan, C.J. Bruns

11:00 038. Investigation of electrode effect on SMOX sensor operation. **S. Astle**, K. Valeti, K. Rafiq, A. Staerz

THURSDAY AFTERNOON

Advances in Bioanalytical Chemistry for Emerging Contaminants

Alvarado Salon F

Cosponsored by ENVR
C. Feng, *Organizer, Presiding*

1:00 Introductory remarks.

1:05 039. In-depth literature review focused on PFAS (per- and poly-fluoroalkyl substances) chemicals and PCB's (polychlorinated biphenyls). **S. Begum**

1:30 040. Development of two fluoride-responsive fluorescent probes to identify PFAS-degrading bacteria with single-cell resolution. **A. Weizenbeck**, D. Domaille

1:55 041. Understanding pesticide exposure between migrant and resident birds: Simultaneous analysis of neonicotinoid and diamide pesticides in avian biosamples. **B.R. Blackwell**, M.J. Anderson, K.A. Luchini, C. Farrell, A. Janik, E.B. Cohen, J.M. Fair, S.A. Hamer

2:20 Break.

2:35 042. Environmental microplastics promote colon tumorigenesis via Piezo1–calcium–Ros signaling and hypoxia-induced metastatic pathways. **X. Xue**, L. Goodla

3:00 043. Quantitative analysis and identification of micro and nanoplastics in the hemisphere of a human brain. **M. Garcia**, L. Barela, E. Phan, R. Liu, E. El Hayek, B. Bleske, N. Adolphi, D. Gallego, M. Campen

3:25 044. Quantitative LA-ICP-MS imaging of metal distributions in lung and colon disease. **R. Liu**, M. MazloumiBakhshayesh, A. Bolt, X. Xue, C. Feng, M. Campen

Energy and Solar Technologies

Alvarado Salon C

Cosponsored by ENFL
B. R. Wygant, *Organizer, Presiding*

1:00 Introductory remarks.

1:05 046. Methods of Li-ion battery cathode processing and subsequent material separation by froth filtration to improve collection of cathode active material. **B.R. Wygant**, J. Pillars, D. Rademacher, K. Leung

1:30 047. Alternative pathways for strengthening PV thin glasses. **J.M. Rimsza**, T. Diebold, K. Strong

1:55 Break.

2:10 048. Use of carbonyl as an infrared reporter for probing the nature of charges in oligo(*p*-phenylene)s. **J. Yan**

Functional Materials for Energy Transduction

Alvarado Salon G

Cosponsored by PHYS
J. Olivier, J. Rack, *Organizers, Presiding*

1:00 Introductory remarks.

1:15 049. Transient control of dimensionality in supramolecular assemblies via fuel-driven donor–acceptor complex formation. **I. Tsironi**, S.L. O'Leary, J. Maleszka, X. Xia, Y. He, J. Watt, J. Olivier

1:40 050. Electrodeposited NiFeCo + Tb and Dy for enhanced magnetostrictive properties and soft magnetism. **M. Faltas**, J. Pillars, M. Rodriguez, N. Gurule, P. Finnegan, T. Monson, G. Subramania

2:05 051. PEG-stapled chiral PDI supramolecular polymers for directional charge and spin transport. **J. Maleszka**, I. Tsironi Tzinious, V.A. Paulino, J. Olivier

General Nuclear Chemistry

Alvarado Salon DE

Cosponsored by NUCL
A. Andersson, D. R. Porterfield, R. Pulido, *Organizers, Presiding*

1:00 Introductory remarks.

1:10 052. ASTM, ISO, and IEEE standards organization update. **D.R. Porterfield**

1:30 053. Applications of scanning tunneling microscopy in heavy element studies. **B.R. Heiner**, M.F. Beaux

1:50 Break.

2:10 054. 19F NMR to quantify 235U enrichment in UF6. **J. Davis**, H.T. Fabich, M.S. Conradi, K. Polack, K.J. Fritzsching, J. Richards, J. Hobby, P. Magnelind

2:30 055. Synthesizing the pertechnetate/perrhenate linked actinide compounds towards understanding role of M-TcO_4 connectivity in Tc-99 mobility during spent nuclear fuel reprocessing. **M. Shohel**, J. Bustos, I. Colliard, M.D. Nyman

2:50 056. AI-enhanced distributed optical fiber based monitoring system for spent nuclear fuel storage applications. **P. Ohodnicki**, K. Naeem, E. Sarcinelli, K. Denslow, R. Meyer

3:10 057. Ab initio study of polymorphism and phase transitions in $Na_2U_2O_7$. **E. Kim**

Materials for Electrochemical Energy Storage and Conversion

Alvarado Salon A

Cosponsored by ENFL
D. Chen, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 058. Barium niobate perovskite catalysts for oxidative and electro-oxidative methane transformation. **F. Garzon**, L. Denoyer, K. Troche, K. Ramaiyan

1:35 059. Harnessing static and dynamic disorder for solid-state ion transport. **A. Maughan**

2:05 060. Stable room temperature sodium sulfur batteries via in-situ crosslinked functional gel polymer electrolytes. **H. Nguyen**, S. Wei

2:25 Break.

2:40 061. Enhancing performance of an archetypal organometallic complex for aqueous redox flow batteries. **N. Holubowitch**, A. Burghoff

3:10 062. Enhancing electrochemical performance of P2-type $Na_{0.67}MnO_2$ cathode material through Al and Mg doping for sodium-ion batteries. **M. Ahangari**, **M. Zhou**, **H. Luo**

3:30 Break.

3:40 063. Primitive cubic cation-disordered niobium tungsten oxides. **B. Raji-Adefila**

4:00 064. Partially cation-disordered zigzag-type framework for advanced Mn-based Li-ion battery cathodes. **Y. Wang**, W. Choe, D. Chen

Sensor Technologies

Alvarado Salon B

Cosponsored by PHYS
S. Percival, *Organizer, Presiding*

1:00 Introductory remarks.

1:05 065. Fabricating ordered arrays of functionalized nanoparticles via SECCM for applications in electrochemical biosensing. **K. Osoro**, C.M. Hill

1:30 066. Toward next-generation of semiconducting metal oxide gas sensors through the cross-pollination of sensor excitation and data analytics. **K. RAFIQ**, C. Crabtree, R.A. Potyrailo, C. Kostelecky, A. Staerz

1:55 Break.

2:00 067. Effect of carbon-nitride dot emitting species evolution on fluorescence-based sensing and differentiation. **J.K. Grey**, E. Westphal, K. Ghosh

2:25 068. Automated gas mixing system for long-term degradation study of semiconducting metal oxied based gas sensors. **C. Crabtree**, K. Rafiq, K. Valeti, S. Astle, A. Staerz

THURSDAY EVENING

Opening Reception Poster Session

East Atrium

M. Christian, A. S. Edgar, E. Eke, M. Houck, L. J. Whalen, *Organizers*

6:00 - 8:00

045. Controlled directional emissivity via 2-D waveguides arrays. **G.C. Gee**, R. Reyna, M.J. Risely, Y. Dong, B. Burckel

069. Analyzing the role of the N-terminal unstructured tail on MabA activity and interactions. **T.B. Jeter**, M.L. Johnston

070. Evolutionary conservation of electropositive surfaces on the membrane-binding C2 domains of synaptotagmin-like protein 4. **V. Raju**, N.L. Chon, C.S. Miller, H. Lin, J.D. Knight

071. Quantification of heterochiral duplexes using molecular dynamics. **A.J. Baten**, A. Mishra, M.R. Lakin, W.P. Bricker

072. Title: Establishing structural parameters of the 5'-GUAC sequence as an RNA motif. **Y. Barache**, V. Nguyen, O. Lear, M.J. Resendiz

073. Predicting liquid-liquid phase separation of neurodegenerative proteins in presence of RNA. **K. Welch**, A. Shakya

074. Fluorescent polarization is superior to BIOMOL® for measuring RecA binding affinity. **E.L. Scott**, R.L. Moore

075. Calibration matters: Refining cell density and imaging for reliable dose-response data. **N.M. Dyson**, C. Collom

076. Development of a translation recorder system in living cells. **H. Hirose**, T. STASEVICH

077. Training innate immunity: Towards a pathogen-agnostic vaccine. **R. Kidner**, A. Romero, A. Shanker, J. Kubicek-Southerland

078. Designing methamphetamine hapten vaccines to combat chronic substance abuse disorder. **M.K. Whittington**, C. Rice, B. Tran, M. Marty, N. Lee

079. Investigating the reactivity between thiol- and carbonyl-containing compounds. **M. Paris**, S.J. Karpowicz

080. Competitive reactivity of ascorbate and taurine related molecules toward reactive oxygen species. **N. Nanjo**, S.J. Karpowicz

081. Sustained linalool realeasing polyvinyl alcohol/gellan gum hydrogel for infectious burn wounds: Characterized *in-vitro*. **F. Rashid**, **Q. Faheem**, M. Ikram

082. Understanding the substrate flexibility of the graspetide synthetase, MdnC. **G. Kyei Boateng**, M. Walker

083. Preliminary investigation on brain metabolic alterations induced by intermittent fasting. **T. Jiang**, C. Wang, J. Tandoy, M. Liu, C. Feng

084. Parachute: A soft landing from an introdcutory STEM course facilitates future student success. **J.L. Stafford**, K.J. Ho, A. Ray, S. Knottenbelt

085. Heating up chemistry education with thermal imaging technology. **S.J. Donnelly**

086. Community cultural wealth as a lens for understanding linguistic capital of latine students at an HSI. **N. Chapuma**

087. Intersection of Community Cultural Wealth and STEM resources as Indicators of border crossing in the chemistry classroom. **T. Adesunloye**

088. Biomimetic, controllable synthesis of calcium carbonate via polyphenol-mediated crystallization: Implications for CO_2 mineralization. **L. Shahriari**, S. Eon Han, S. Han, M. Hojati, S. Kim

089. Impacts of chlorination on antibiotic resistance in treated wastewater effluent discharges and receiving irrigation canals. **A. Sharma**, L. Ramadan, M. Harb

090. Hydrodeoxygenation (HDO) of pinyon-juniper (PJ) and feather reed grass (FRG) bio-oil blends: Evaluating process conditions and catalyst performance. **A. HLORPEY**, F.A. Agblevor

091. Advancing detection of per- and polyfluoroalkyl substances via indirect solution analysis with desorption electrospray ionization. **T.M. Griffus**, N. Bays, S. Kruse, M. Shohel, J. Kustas, A. Benally, R.D. Davis

092. Environmental transformation and toxicological impacts of metformin mediated by photocatalysts and organic matter. **R. Khan**, J. Regalado, M.I. Kanaththage, P. Patidar, G. Rubasinghege

093. Investigating the mosquito repellent properties of essential oils from hedge apple and guayule. **J. Brazil**, A. Guillory, H. Luker, I. Hansen, C.E. Brewer

094. Membrane distillation for produced water desalination: Understanding membrane property-solution chemistry relationships. **S. Parajuli**, K.G. Hernandez, N. Sharp, A. McGaughey

095. Catalyzing plastic degradation: Novel mechanochemistry treatment for sustainable plastic waste management. **J. Zhang**

096. Investigating biocrusts growth on abandoned uranium mine soil. H. Stoner, E. Saville, A. Antoninka, **J.C. Ingram**

097. Physicochemical and toxicological profiling of respirable metal, Nonmetal and aggregate mine dust. **M.I. Kanaththage**, K. Macias, G. Rubasinghege, P. Roganchi, M. Rezaee

098. Mineral formation and surface chemistry alterations affect mixed metal sorption with filamentous fungi for bioremediation applications. **J.A. Bartholomeusz**, C. Whitmore, G. Flores, C. De Vore

099. Mixtures relevant to Titan's lakes: A molecular dynamics study. **M. Brand**, G.E. Lindberg, A. Engle, J. Hanley

100. Critical points in catalysis: Analyzing critical point motion in the presence of external electric fields. **H.A. Redmon**, A. Morgenstern

101. Large-scale computational modeling of fluoroalkyl radical EPR spectra. **C. Bosgraaf**, M. Zumtobel, I. Spackman, S. Vyas

102. Controlling unoccupied molecular orbital stability using external electric fields. **N. Maruska**, H.A. Redmon, A. Morgenstern

103. Computational and experimental mechanistic study of turn-on luminescence of amyloid-beta targeting oligomeric p-phenylene ethynylenes. **B. Fetrow**, E.Y. Chi, W.P. Bricker, J. King

104. Modeling the robustness and efficiency in photosynthetic light harvesting networks. **Z.E. Armijo**, W.P. Bricker

105. Theoretical and computational studies on metalloporphyrin magnetic circular dichroism response. **J. Brink**, S. Smith, J. Rack

106. Applying critical point positions for enzyme design: Kemp eliminase directed evolution. **K. Ly**, H.A. Redmon, A. Morgenstern

107. How understanding enzyme – substrate motion can guide smarter drug design. **L. Ongboja**, S.J. Karpowicz

108. Structural, electronic, and optical properties of dietary flavonoids: Implications for Huntington's Disease pathology. **K.M. Garcia Homs**, N. Saikia

109. Molecular dynamics of methanium and ethanium in methane and ethane at Titan conditions. **W.E. Rosen**, A. Hardin, M. Salvatore, G.E. Lindberg

110. Python-driven benchmarking of EPR parameters for fluorinated species: using spin traps to investigate degradation mechanisms of diverse PFAS molecules. **M. Zumtobel**, C. Bosgraaf, I. Spackman, S. Vyas

111. 2D fluorescence of Phycocyanin bioconjugation and its impact on light harvesting. **B. Shakespeare**, T. Holmes, C. Koch, J. Dean

112. pH- and oxygen-sensitive photochemistry of a model dipyrrole in solution. **J.S. Meikle**, S. Archer, D. Newbold, C. Williams, T. Clark, A. Fisher, M. Prater, J.C. Dean

113. Structure-based virtual screening of ligands targeting P-glycoprotein to mitigate vitamin D deficiency. **S. Garlanka**, G. Sharma

114. Advanced analytical techniques for isolation and quantification of micro(nano)plastics in human cerebrospinal fluid: implications for brain waste clearance disorders. **S. Patil**, M.E. Park, J. Kingston, M. Garcia, R. Smith, M. MazloumiBakhshayesh, R. Liu, T. Howard, J. Gross, J.

Gonzalez-Estrella, S. Noor, K. Bhaskar, B. Shuttleworth, C. Cole, M. Campen, A. Carlson, E. El Hayek

115. Identification of potential molecular interference of lipids and micro(nano)plastics during pyrolysis gas chromatography-mass spectrometry analysis. **R. Smith**, M.E. Park, S. Patil, M. Garcia, R. Liu, E. Descher, L. Barela, M. MazloumiBakhshayesh, M. Campen, E. El Hayek, J. Kingston

116. Probing supramolecular complexes and hierarchical organic structures with nano-FTIR spectroscopy. **G.P. Dorce**, W.M. Takele, M.J. Holzmann, K. Ghosh, J.K. Grey, T. Habteyes

117. Nanoscale control and elucidation of Stark effect mechanisms in P3HT-F4TCNQ blends with Nearfield spectroscopy. **W. Abebe**, **T. Habteyes**

118. Molecular optomechanical coupling in plasmonic nanocavities. **B. Gao**

119. Molecular optomechanics as sensor for vibrational pumping. **J. Damoah**

120. Identifying ice grain orientation via Raman spectroscopy: Perceived spectral shift based on crystal rotation. **M. Feduschak**, K. Hammonds

121. Development of a microplate-based starch-iodine assay for hydrogen peroxide quantification in biological samples. **H. Nixon**

122. Proteomics and sea star wasting disease. **E. Rosenkranz**

123. Flavoring chelation properties influence the quantity of metals in vaping aerosols. **A. Perez**, C. Collom

124. Tuning diketopyrrolopyrrole near-infrared emission through molecular weight and nanoparticle size. **A.C. Fritz**, N. Gill, R. Posey, J. Tropp

125. Regulating radical flux in frontal polymerization. **D. Ivannikava**, J.J. Lessard

126. Branching effects on associative covalent adaptable networks. **F. Lombardi**, J.J. Lessard

127. Synthesis and characterization of Thienoisoindigo (TIG) oligomers and polymers featuring aggregation-enhanced emission. **C.B. Cashman**, R. Posey, N. Gill, J. Tropp

128. Chemical upcycling of polydicyclopentadiene (pDCPD) via dynamic imine crosslinking. **L. Shahriari**, C. Biju, L. Elam, H. Fowler, S.C. Leguizamon, S. Kim

129. Enzyme-degradable peptide hydrogels as smart biomaterials for triggered drug release. **S. Salika Dulanjali**, J. Olivier

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

131. Green solvent and froth floatation to enable the separation of lithium-ion battery cathodes. **J. Pillars**, B.R. Wygant, D. Rademacher

132. Comparative analysis of efficient neuropeptide extraction methods for quantitative peptidomics and application. **A.K. Apawu**

133. Optical detection and discrimination of PFAS using Conjugated Polyelectrolytes. **B. Alfaro**, J. Tropp

134. Computational simulations of bispecific aptamers for ovarian cancer diagnosis. V. Sharma, **G. Sharma**

135. Detecting heart failure before it strikes: in silico analysis of aptamer-mediated GPNMB protein detection in congestive heart failure (CHF). S. Vedagiri, **G. Sharma**

136. Computational modeling of calprotectin targeting aptamers as a Crohn's disease biomarker. **G. Sharma**

137. CD19-targeted chimeric antigen receptor (CAR) T cell therapy in multiple sclerosis. **M. Govind**, G. Sharma

138. Computational simulation of progranulin for blood-based detection of Parkinson's disease up to 7 years before symptom onset. **K. Madapathi**, S. Madapathi, G. Sharma

139. Studying an underexplored target in mycolic acid biosynthesis. M. Malin, S. Morrison, F. Hennessy, T.B. Jeter, **M.L. Johnston**

140. Targeting MabA in mycobacteria: Docking-based identification and enzymatic validation of novel inhibitors. **F. Hennessy**, M.L. Johnston

141. Small molecule drug discovery and cryptic binding pocket detection in human Doppel. **J. Sanchez**, W. Guo, Y. Li

142. In silico design and optimization of ROR1 T-cell constructs targeting non-small cell lung cancer. **R. Das**, G. Sharma

143. Structure-guided design of proteolysis-targeting chimeras (PROTACs) for the selective ubiquitin-mediated degradation of glycogen synthase kinase-3 beta (GSK-3β) against Alzheimer's diseases. **M. Kumari**, G. Sharma

144. Discovery of a novel compound with potential to overcome glioblastoma drug resistance. **H. Zhang**, Y. Li

145. Zero liquid discharge of produced water via an integrated membrane distillation and crystallization process. **G. Fernandez**, Z. He, J. Kessie, J. Yu

146. Electrochemical studies of pentacyanodimethylsulfoxide ferrate(II) and tetracyanobisdimethylsulfoxide ferrate(II): A novel example of sulfoxide isomerization on iron(II). **S.B. Adekoya**, J. Rack

147. Simulations of hierarchical dynamic electroactive nanomaterials. **R.S. Wilson-Kovacs**

148. Optimization of the RecA+ strain. **D. Dodd**, M. Dyson

149. Ligand symmetry-driven control of excited-state dynamics in related polypyridyl iron(II) complexes. **J. Knouse**, E. Quartey, S. Smith, J. Brink, J. Rack

150. Pincer ligand design for molecular catalyst facilitating ammonia oxidation. **M. Crotzer**, M. Denman, M.T. Mock, S.I. Johnson

151. Conformation of six-membered vanadium chelate rings. **K. Jenkins**, S.A. Markham, A. Gibson, C.C. McLauchlan, D.C. Crans

152. Towards morphology control of strongly confined $CsPbBr_3$ perovskite quantum dots. **M. Atteberry**, Y. Dong

153. Varying selectivity in C-F activation of aryl fluorides as a result of catalyst modifications in bis-bidentate N-heterocyclic carbene nickel complexes. **A.C. Garcia Alvarez**

154. Reactivity of carboranyl boranes. **K. Vashisth**, S. Dutta, M. AKRAM, C. Martin

155. Divergent outcomes in the reactions of boroles with Michler's ketone and thioketone. **D. Alwis**, A. Begum, C. Martin

156. Müller *versus* Gutmann–Beckett for assessing the Lewis acidity of boranes. **S. Ranasinghe**, Y. Li, M. Andrews, M. AKRAM, R. Thornton, C. Martin

157. Dearomative C2-borylation of indoles. **A. Begum**, M. AKRAM, C. Martin

158. Magneto-optical activity of *cis*- and *trans*-substituted metalloporphyrins. **S. Smith**, J. Brink, J. Rack

159. Magneto-optical activity of fluorinated and non-fluorinated free base porphyrins. **B.U. Rajapakshe**, S. Carrillo, J. Rack

160. Investigation of magneto-optical properties of metalloporphyrins in solution vs solid state. **M.G. Saeed**, B.U. Rajapakshe, S. Smith, J. Rack

161. Photoisomerization and ligand field modulation in Fe(II) complexes. **J.D. Velasco**, J. Brink, J. Rack

162. Mechanistic insights into photoracemization of aryl sulfoxides. **E. Quartey**, S. Smith, J. Brink, J. Rack

163. Synthesis and characterization of iron(II) spin-crossover complexes comprising pyridine-thioether ligands. **S.B. Siriwardane**, J. Rack

164. Synthesis and characterization of Mono-ruthenium complexes with hypoxanthine and chiral Thione ligands. **T. Phan**

165. Lessons from metals-containing drugs in diagnostic, and theranostic applications for future development of metal-containing therapeutics: Vanadium compounds for intratumor administration. **A. Miller**, D.C. Crans

166. Structure-property relationships in Sb^{3+}-doped A_2InCl_5-H_2O and A_3InCl_6: Effects of cation substitution, dimensionality, and temperature. **A. Blackbear**, D. Retzloff, M. Wallace

167. Exploring thermochromism in iron-based halide compounds: Structure, stability, and optical tuning. **K. Butler**, **A. Blackbear**, C. Kooy, M. Wallace

168. Chemical vapor deposition of niobium and tantalum oxides using a custom-built system. **H. Garland**, S.K. Hurst

169. Biocatalytic aza-Michael addition of aromatic amines to enone using α-amylase in water. **S. DUTT**

170. Escape from flatland: Pericyclic reactions and rearrangements of Diazofluorene with Biarylcyclooctynes for the generation of helicene-like phenanthro-pyrazoles. **A. Ojha**, E. Das, X. Lin, B. Gold

171. Optimization of boride reduction of 3,5-disubstituted isoxazoles. **N. Beitle**

172. Cross carbonyl-olefin metathesis (XCOM) of unactivated olefins. **J. Wu**, M. Vargas-Penalver, T.H. Lambert

173. Bioanalytical profiling of Taraxacum kok-saghyz reveals tissue-specific biomarkers with therapeutic potential. **M. Tan**, D. Swiger, C. Jeffrey

174. Advances in nanocarrier systems for Dermatologic transdermal drug delivery: A chemical and molecular review. **A.D. Parga**

175. Identification and characterization of FKBP52-specific inhibitors for the treatment of prostate cancer. **N. Sahragardan**, M. B. Cox, R. D. Koyani, Y. Li

176. AI-Driven FTIR for lactose quantification: A powerful alternative to conventional analytical methods. **N.L. Torres**, V. Ramos, I. Salmeron Ochoa, J.M. Napoles Duarte, R. Orozco Mena, S. Perez Vega

177. Development of physics-informed and uncertainty-aware neural network force-fields for coarse-grained polymers. **P.G. Sahrmann**, B.W. Hamilton, K. Barros, B.T. Nebgen

178. Signal from the noise: Automated spectral figure extraction for systematic literature review in python. **I. Spackman**, S. Vyas

179. Machine-learned electronic structures for biological systems. **E.M. HALIBA**, W.P. Bricker

180. Design and synthesis of green ionic liquids for solid polymer electrolytes. **K. Bridge**, C.C. Browder

FRIDAY MORNING

Biological Chemistry: Biomolecular Condensates

Alvarado Salon G

Cosponsored by BIOL
A. Shakya, *Organizer*
M. Walker, *Presiding*

8:00 Introductory remarks.

8:05 181. Fold, bridge, condense: Exploring how phase-separating proteins reshape chromatin through coarse-grained simulations. **U. Kapoor**

8:30 182. The liquid material properties of a conserved chromosomal interface. S. Gordon, L. KURSEL, K. Patterson, A. Rodriguez, Y. Gu, K. Corbett, C. Lee, J. Brasch, **O. Rog**

8:55 183. PRDM paralogs control neural crest development through association with nucleosomes. **L.C. Shull**

9:20 Break.

9:30 184. Smart nucleic acid chaperones: phase-separating intrinsically disordered proteins for accelerating nucleic acid hybridization reactions. **T. Diez Perez**, A. Tafoya, D. Peabody, A.P. Shreve, M.R. Lakin, N. Carroll, G. Lopez

9:50 185. Elastin-like polypeptide condensates: characterization and predictive modeling of phase behavior. **A. Quintana**, G. Lopez, N. Carroll

10:10 186. Protein unfolding thermodynamics as a measure of phase separation propensity. N. Rana, **M. Kayser**, R. Kodirov, A. Shakya, J. King

10:30 Break.

10:40 187. Selective uranium preconcentration through molecular recognition and protein-driven phase separation. **A. Tafoya**, C. Yazzie, A. Apodaca-Sparks, A. Ali, D. Peabody, J.M. Cerrato, G. Lopez

11:00 188. Investigating the phase separation properties of canonical high mobility group (HMG) proteins. **E. Haes**, A. Shakya

11:20 189. Decoding KIF14's mechanochemical cycle step-by-step. **A. Htut**, S. Hernandez, S.R. Atlas

General Computational Chemistry

Alvarado Salon DE

Cosponsored by COMP
Y. He, *Organizer, Presiding*

8:00 Introductory remarks.

8:05 190. Driving forces of RNA condensation: Coarse- grained modeling with explicit Mg2+. S. Li, **J. Chen**

8:25 191. Fast sampling of protein conformational transitions. M.A. Sauer, S. Mondal, **M. Heyden**

8:45 192. Exploring "constrained" protein conformations with physics-guided artificial intelligence. Y. liu, Y. Wang, Z. Yu, G. Lin, W. Jiang, **M. Chen**

9:05 Break.

9:20 193. Enhancing the generative capabilities of ShapeGMM via minimization and analytic Hessian evaluation. G. Copland, **M. McCullagh**

9:40 194. Integration of nisin into biological membranes. **R. Sheridan**

9:55 195. Generative AI for molecular simulations: From coarse-graining to rare event discovery. **y. wang**

10:15 196. Mismatch binding molecules as therapeutic agents for repeat expansion neurodegenerative diseases. **N. Saikia**

10:35 Break.

10:50 197. Computer-aided drug design tools for polypharmacology in multi-target drug discovery. **K. Elokely**

11:10 198. Metalloproteins regulate net charge to control electron transfer energetics. **M.J. Guberman-Pfeffer**

11:30 199. Peptide engineering targeting the SSX1–SS18 fusion protein via BindCraft. **E. Hendrix**, Y. He

General Inorganic Chemistry

Alvarado Salon C

Cosponsored by INOR
D. C. Crans, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 200. Breaking strong bonds using molybdenum enzymes. **M.L. Kirk**

8:35 201. Thorium and uranium: Elements of opportunity in actinide organometallic chemistry. **J.L. Kiplinger**

9:05 Break.

9:20 202. Development and application of vanadium complexes for treatment of diabetes and cancer: Specific phosphatase inhibitors and other active antiproliferative complexes. **D.C. Crans**, x. Yang

9:50 203. Diversification of molybdenum(III) precursors for vapor-phase materials growth. **T.M. Currie**, L. McElwee-White, T. Jurca

10:20 Break.

10:35 204. Electronic structure differences between the mitochondrial amidoxime reducing component and sulfite oxidase. **J. Yang**, M. Struwe, K. Kolanji, J. Mengell, A. Scheidig, B. Clement, M.L. Kirk

10:55 205. Unveiling the reactivity of bis(1-methyl-*ortho*-carboranyl)borane: Hydroborations and beyond. **M. AKRAM**, C. Martin

11:15 206. Harnessing metal acetylides for Vinylborane synthesis. **R. Thornton**, C. Martin

11:35 207. Design of experiments (DOE) methods for the synthesis of gold nanoparticles in the presence of catechin. I. Subuloye, D. McCoy, L. Lucero, **M. Watzky**

AI/ML Approaches to Chemistry and Materials Modeling

Alvarado Salon F

Cosponsored by COMP
D. Robinson Brown, S. Tretiak, *Organizers, Presiding*

9:00 Introductory remarks.

9:05 208. Adventures in latent space: Physics-based design of dynamical potentials. **S.R. Atlas**

9:50 209. Machine-learned electronic structure of biomolecules. **W.P. Bricker**

10:20 Break.

10:40 210. Machine learning of bonding character and quantum entanglement in diatomic molecules. **S. Samuels**, C. Baxter, S.R. Atlas

11:10 211. From first principles to AI: evolving tools for materials discovery. **I. Matanovic**

11:40 Break.

11:50 212. Uncovering the role of critical bonds in the thermomechanical response of Zn_2(1,4-benzenedicarboxylate)$_2$(1,4-diazabicyclo[2,2, 2]octane) using ab initio simulations and physics-constrained neural network. **R.A. Chowdhury**, B. Ghose, D. Choudhuri

Chemical Separations

Alvarado Salon A

Cosponsored by PHYS
G. Nagy, *Organizer, Presiding*

9:00 Introductory remarks.

9:05 213. Isotopic shifts in high-resolution ion mobility separations. N. Roberts, D. Williamson, **G. Nagy**

9:30 214. Advancing spatial metabolomics with on-target chemical derivatization, ion mobility, and *in-silico* prediction of derivatized analytes. D. Veličković, A. Moreno-Pedraza, K. Zemaitis, T. Zeng, M. Veličković, H. Vandyk, X. Zheng, **C.R. Anderton**

9:55 215. Adduct matters: Differences in small molecule ionization across mass spectrometry platforms. **M. Odenkirk**, J.M. Chaparro, C. Broeckling, J. Prenni

10:20 Break.

10:35 216. Ion mobility-assisted sequencing of protein ions. **N. Borotto**

11:00 217. An in-depth single-cell proteome every 5 min or less with multicolumn LC system. **C. Wang**, H.L. Lin, S. Huang, T. Truong, X. Xie, G. Haynie, K. Triggs, Z. Chang, R. Kelly

11:25 218. Novel applications of gas-phase separations in structures for lossless ion manipulations (SLIM). **S. Garimella**, C. Harillal, Y. Ibrahim

General Analytical Chemistry

Alvarado Salon B

Cosponsored by ANYL
E. Heider, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 219. Enhanced approaches to materials compatibility testing: analytical investigations of interfacial and gas phase chemistry. **N. Bays**, D. Schafer, T.M. Griffus, A. Benally, P.R. Tumminello, T.F. Babuska, R.D. Davis

9:30 220. Flow cytometric analysis of lipo-beads for the detection of emerging cardiovascular biomarker: phospholipase A_2. **D. Senavirathna**, B. Phelps, M. Broton, M.E. Piyasena

9:55 Break.

10:10 221. Acoustic focusing based separation and purification of heavy metals adsorbed microplastics in the aquatic environment. **N.A. DeSilva**, M.E. Piyasena

10:35 222. Monitoring chemical indicators and harmful algal blooms in a large arid-region Lake. T. Hill, C. Bell-Hunley, **E. Heider**

11:00 Break.

11:15 223. Insitu optical endpoint detection for high accuracy parylene film deposition. **S. Larson**, A. Mings, K. Coombes, J. Norris

General Polymer Chemistry

Weavers Room

Cosponsored by POLY
H. Dedmon, *Organizer, Presiding*

9:00 Introductory remarks.

9:05 224. Impact of hydrogen oversaturation on filler-elastomer adhesion: Insights from molecular dynamics simulation. **M. Wilson**, I. Winters, A.L. Frischknecht

9:30 225. Encapsulating Grubbs type catalysts for frontal ring opening metathesis polymerization. **O. Davydovich**, S.C. Leguizamon, B. Jones

9:55 226. Effects of linking chemistry on the stability and performance of triblock copolymer anion exchange membrane. **M.L. Carroll**, A.M. Herring

10:20 Break.

10:35 227. Exploring new frontiers in electrochromic conjugated polymer synthesis and molecular design. **R.M. Pankow**

11:00 228. Rational design of conjugated polymer nanoparticles with bright emission in the NIR-II. **N. Gill**, A.C. Fritz, R. Posey, J. Tropp

FRIDAY AFTERNOON

Advances in Spectroscopy

Alvarado Salon B

Cosponsored by ANYL
J. Harper, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 229. ^{19}F NMR difference spectra correlate TRPM8 receptor protein dynamics, bound ligand structure and cellular function. M. Mebrat, D. Luu, **W.D. Van Horn**

1:30 230. The power ^{19}F NMR prediction using DFT methods to accelerate NMR structure elucidation. **N.C. Gonnella**, R. Ghosh, G. Valdivia-Berroeta, D. Xin

1:55 231. Complete and accurate structure determination from a single NMR experiment. **J. Harper**, E. Heider

2:20 Break.

2:30 232. From fleeting states to therapeutics: New perspectives in protein-RNA binding. **C. Taylor**, J. King

2:55 233. Variable repetition rate for long-timescale detection of biomolecular dynamics. **Q. Le**, J. King

3:20 Break.

3:30 234. Single-molecule correlation spectroscopy to study biomolecular dynamics. C. Taylor, Q. Le, **J. King**

3:55 235. Excited triplet state zero-field splitting in a ligand-to-ligand charge transfer complex. **J. Mengell**, S. Gao, C. Mangione, M. Yadav, D. Kersi, J. Yang, S. McGill, D.A. Shultz, M.L. Kirk

Biological Chemistry: Biomolecular Condensates

Alvarado Salon G

Cosponsored by BIOL
A. Shakya, *Organizer*
M. Walker, *Presiding*

1:00 Introductory remarks.

1:05 236. Imaging single mRNA translation dynamics in the context of biomolecular condensates. **T. STASEVICH**

1:30 237. Lipid membrane templated misfolding, self-assembly, and phase separation of intrinsically disordered tau protein. J. Majewski, E. Jones, C. Vander Zanden, J. Biernat, E. Mandelkow, **E.Y. Chi**

1:55 238. Exploring the unique structural features of the 5'-GUAC sequence motif. **M.J. Resendiz**

2:20 Break.

2:30 239. Creating an integrated anti-CRISPR system to harden bioeconomy organisms against CRISPR editing. **K. Butler**

2:50 240. Structural and kinetic studies of nucleic acid and intrinsically disordered chaperone complexes for bioengineering applications. **J. Belchak**, R.P. Hjelm, W. Leite, H.M. O'Neill, N. Carroll, K.L. Weiss, G. Lopez

3:10 241. Label-free fluorescence microscopy reveals multiphase organization in biomolecular condensates. B. Acharya, **S. Castillo**, R. Kodirov, A. Shakya

3:30 Break.

3:40 242. Liquid-liquid phase separation modulated ribozyme activity. **Y. Gautam**

4:00 243. Modeling a mitochondrial protein implicated in cell death: Structural consequences of mutations in the transmembrane domain of ATP synthase. **S. Crotzer**, Q.(. Wang, S.C. Pias

Chemical Education

Alvarado Salon C

Cosponsored by CHED
D. Habel-Rodriguez, J. L. Stafford, *Organizers, Presiding*

1:00 Introduction - 5 minutes.

1:05 244. Expanded course-based undergraduate research experience (ECURE) in chemistry curriculum. **K.J. Ho**

1:25 245. Small steps, big impact: Implementing course-based undergraduate research experiences in online introductory chemistry labs. **C. Wang**

1:45 246. A pre-CURE implementation in a large General Chemistry lecture course. **D. Habel-Rodriguez**, K.J. Ho

2:05 247. Exploratory research as an effective pedagogical tool at two-year college institutions: Reaching learning objectives for the biotechnology courses via class-embedded cancer research project. **P. Filipczak**

2:25 Panel discussion - 10 minutes.

2:35 Break - 10 minutes.

2:45 Introduction - 5 minutes.

2:50 248. Teaching organic chemistry in general chemistry: Why not?. **S.J. Donnelly**

3:10 249. From cookbook to critical thinking: Transition to a guided inquiry approach for second semester general chemistry laboratory. **A. Johnson**, K. Addamane

3:30 250. Rotating first-semester general chemistry students towards polarimetry. **S.J. Donnelly**

3:50 251. Exploring luminescent and colored halide materials: An adaptable, inquiry-based lab framework for undergraduate chemistry courses. A. Blackbear, N. Robey, **M. Wallace**

4:10 Panel discussion - 10 minutes.

Chemical Separations

Alvarado Salon A

Cosponsored by PHYS
G. Nagy, *Organizer, Presiding*

1:00 Introductory remarks.

1:05 252. Rare earth solvent extraction using a tunable vinyl phosphonic acid scaffold. **T. Mallos**, A.A. Kuvayskaya, A. Sellinger, M.P. Jensen

1:30 253. Electrochemically-driven separation of tellurium from spent thin-film photovoltaic solar panels. **A. Mukhopadhyay**, M. Shi, D. To, H. Rollins, D.M. Ginosar, H. Jin

1:55 Break.

2:10 254. Size exclusion chromatography coupled to charge detection mass spectrometry via Hadamard transform multiplexing. **J.D. Sanders**, M. Marty, B. Tran

2:35 255. Characterizing the effects of PFAS binding on protein structure and stability. **E.O. KUKOYI**

3:00 256. Leveraging phase separation dynamics in silica-alkali glass for efficient rare earth element extraction. **B.W. Juba**, M. Shohel, K. Strong, T. Diebold, J. Phillips, N. Bays, S. Kruse, J. Kustas

General Computational Chemistry

Alvarado Salon DE

Cosponsored by COMP
Y. He, *Organizer, Presiding*

1:00 Introductory remarks.

1:05 257. Simulating the modulation of amyloid formation and inhibition by small peptides. L. Coleman, M. Premathilaka, A. Chesney, **U. Hansmann**

1:25 258. Quantifying charge density rearrangement from external electric fields. L. Epperson, M. Mascarenas, N. Hughes, **A. Morgenstern**

1:45 259. Impact of π-spacers and acceptors on the optoelectronic properties of TPA-derived donor-based dyes: First principles approach. **J.K. Roy**, T. Lafferty, A. Adhikari

2:05 Break.

2:20 260. Molecular insights into kinesin-5 binding to microtubule via TIRF and MD. **W. Guo**, J.E. Sanchez, L. Li, Y. Li

2:35 261. Preliminary modeling and experimental study of bulk ozonolysis kinetics of PFAS. **O. Diaz-Ibarra**, S. Kruse, N.R. Bays, T.M. Griffus, R.D. Davis

2:55 262. Classification using virtual reality reduces false positives and false negatives. **J.H. Kalivas**, H. Redd

3:15 Break.

3:30 263. Revealing complex biomolecular dynamics from smFRET data using Bayesian Nonparametrics. **A. Saurabh**

3:45 264. Computational strategies for the structural design of non-standard peptides: AApeptides. **X. Xia**, Y. He

General Physical Chemistry Gas Capture Technologies

Alvarado Salon F

Cosponsored by PHYS
J. M. Rimsza, *Organizer, Presiding*

1:00 Introductory Remarks Physical Chemistry.

1:05 265. Combinatorically estimating the orbital occupancy of actinides using an entropic approach. **M.F. Beaux**, B.R. Heiner

1:30 266. Accessible, efficient biochemical modeling and experiment design using the Stochastic System Identification Toolkit (SSIT). **A. Popinga**, D. Svetlov, **B. Munsky**

1:55 Break.

2:10 267. Engineering sorbents for noble gas separations at scale: Bridging the gap between benchtop and industry. **M. Hurlock**, K. Krishnan, S. Shin, H. Goettsche, P.K. Thallapally

2:35 268. Enhanced adsorption of trace SF_6 via functionalization of Ni-based metal-organic framework. **N. Gantzler**, J. Geary, J. Harvey, R.E. Sikma, R.A. Reyes, C.E. McKeown, J. Sammon, N.S. Bobbitt, D.F. Sava Gallis

3:00 Break.

3:10 269. Design of azobenzene-containing organic cages for tunable gas separations. H. Root, S. Goodman-Miller, B.M. Addison, **J.M. Rimsza**

General Polymer Chemistry

Weavers Room

Cosponsored by POLY
H. Dedmon, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 270. Effective recycling pathways of commodity polymers enabled by Mechanoradical capture. **A. Cunningham**, M. Hill

1:30 271. Competitive inhibition as a tool to modulate and predict hydrogel properties. **A. Claiborne**, S. Mekcham, O. Lee, M. Hill

1:55 272. Dynamic imine crosslinking for sustainable upcycling of thermoplastics and thermosets. L. Shariari, C. Biju, H.E. Fowler, S.C. Leguizamon, **S. Kim**

2:20 Break.

2:35 273. Optimization and scale-up of the polymerization of Glycoaldehyde-dimer to PDHDO, an eco-friendly and bio-based alternative to petrochemical-based plastics. **R.G. Anderson**, A. Brockway, S.D. Luebben

3:00 274. Leveraging multivalency in dynamic hydrogel design. **M. Rothenberg**, M. Hill

Plenary Lecture with Martin Kirk

Alvarado Salon DE

L. J. Whalen, *Organizer*
A. S. Edgar, *Presiding*

4:30 Introductory Remarks.

4:35 275. Redox active ligands in electronics, photophysics, and biology. **M.L. Kirk**

SATURDAY MORNING

AI/ML Approaches to Chemistry and Materials Modeling

Alvarado Salon B

Cosponsored by COMP
D. Robinson Brown, S. Tretiak, *Organizers, Presiding*

8:00 Introductory remarks.

8:05 276. Nonadiabatic molecular dynamics of nanoscale systems with machine learning. **O.V. Prezhdo**

8:50 277. Prediction of carbon nanostructure mechanical properties and the role of defects using machine learning. J.J. Winetrout, Z. Li, V. Varshney, V. Unnikrishnan, Y. Xu, y. Wang, **H. Heinz**

9:20 Break.

9:40 278. The little 4f electron that could: Density functional and machine learning forcefield methods for cerium at extreme conditions. **B.W. Hamilton**

10:10 279. Finding signal in noisy data-sets: optimizing feature space for small or lower-quality data. **T.A. Purcell**, R. Anjum

10:40 Break.

11:00 280. Hole transport materials for enhanced perovskite solar cell efficiency using DFT and ML. **T. Lafferty**, J.K. Roy

11:30 281. AIMNet2: Foundation neural network potential for molecules and reactions. **O. Isayev**

Biological Chemistry

Alvarado Salon G

Cosponsored by BIOL
M. Walker, *Organizer, Presiding*

8:00 Introductory remarks.

8:05 282. Integrative approaches to unraveling the dynamics of multidomain nitric oxide synthases. **C. Feng**

8:30 283. The chemistry of addiction: A molecular perspective on the interdisciplinary studies of addiction. **D.C. Crans**, C. Chang, D.M. Schlink, D. Roess

8:55 284. Antioxidant role of taurine-related compounds. **S.J. Karpowicz**

9:20 Break.

9:30 285. Cross-linking mass spectrometry for insights into protein structural dynamics. **T. Jiang**, G. Wan, H. Zhang, Y.P. Gyawali, C. Feng

9:50 286. Assessing dietary impact of plastics on sexually dimorphic health outcome and beyond. **S. Phatak**, A. Romero, J. In, M. Campen, E. Castillo

10:10 287. Effect of white band disease on coral tissue lipid composition. **J. Torkelson**, S. LaPeters, N. Eves, K. Brotherton

10:30 Break.

10:40 288. From postulation to proof: Electrochemical synthesis and structural characterization of cordysinin A. **B. Akinlabi**, M. Walker

11:00 289. Site-specific infrared spectroscopic probe of the conformational dynamics in nitric oxide synthases. **R.T. Owopetu**, C. Feng, Y.P. Gyawali, T. Jiang, H. Zhang, M.C. Thielges, S. Singh

11:20 290. Platform for deep mutational analysis and substrate scope of the lasso peptide modifying enzyme. **B.A. Mohammed**

11:40 291. Integrative multi omics reveals gene expression programs in salivary gland adenoid cystic carcinoma through single cell and spatial transcriptomics. **G. Bijukumar**, I. Ebinumoliseh, J. Edwards, K. Hoff, K. Brayer, S. Ness, E.L. Bearer

Environmental and Green Chemistry to Sustain a Healthy Society

Alvarado Salon A

Cosponsored by AGFD
J. M. Cerrato, A. McGaughey, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 292. pH impact on Al-silicate and Pb release in acid mine drainage sediments. **R. Mendes Oliveira**, G. Moreira, A. Saenz Trevizo, A. Ali, A. Brearley, J.M. Cerrato

8:30 293. Investigation of potential elemental contaminants in the Little Colorado River. **A. Trout**, J.C. Ingram

8:55 294. Community collaboration on environmental health studies on Navajo lands. **J.C. Ingram**

9:20 Break.

9:25 295. Metal mobility in post-fire environments: The role of redox between ash and mine wastes. **E. Alcantar-Velasquez**, J.M. Blake, K. Fisher, A. Ali, J.M. Cerrato

9:50 296. Forward osmosis for efficient uranium pre-concentration: Towards low-cost environmental uranium detection. **A. Ropari**, N. Dougan, E. Braun, N. Carroll, J.M. Cerrato, J.J. Lai, G. Lopez, A. McGaughey

10:15 297. Development of bio-based oligoesters from furan units and multiple diols. H. Mewada, **A.M. Schoffstall**

10:40 Break.

10:45 298. Air quality impacts to water quality of atmospheric water harvesting. **A. Mulchandani**, M. Russell, A. Webster, C. Abadam, K. Fisher, S. Campbell, C. Atchley, K. Radius, P. Eisenman, A. Apodaca-Sparks, A. Gonzaga, R. Liu, P. Hudson

11:10 299. Advanced wastewater treatment to address emerging contaminants: Potential of dynamic *versus* conventional membranes to enhance effluent safety in anaerobic MBRs. **L. Ramadan**, M. Harb

11:35 300. Treatment of aqueous phase of bio-oil from catalytic pyrolysis to produce hydrogen and clean water. **E. Valiasil**, **F.A. Agblevor**

Advances in Microscopy

Alvarado Salon F

Cosponsored by ANYL
J. Choe, T. Habteyes, *Organizers, Presiding*

9:00 Introductory Remarks.

9:05 301. Cryo-EM: Revolutionizing our understanding of diseases and drug therapies. **M. Joens**

9:30 302. Cryo-EM structures of the marseillevirus mRNA capping enzyme. **A. Vaiana**

9:55 Break.

10:10 303. XtaLAB Synergy-ED: 3DED/MicroED made easy. **E. Reinheimer**

10:35 304. Fluorescence super-resolution imaging near the quantum limit. **K. Lidke**

Chemical Education

Alvarado Salon C

Cosponsored by CHED
D. Habel-Rodriguez, J. L. Stafford, *Organizers, Presiding*

9:00 Introduction - 5 minutes.

9:05 305. Wise interventions to support student success in General Chemistry. **S. Knottenbelt**

9:25 306. Student experience project: Collaborative exam wrappers. **D. Habel-Rodriguez**, S.Z. Knottenbelt

9:45 307. Elements of success for university general chemistry courses. **K.J. Ho**

10:05 Break.

10:20 308. Understanding the impact of student perceived costs on academic and personal outcomes. **L. Larson**, J. Wright, J. Bui, S. Mooring, **G.A. Rocabado**

10:40 309. Expanding early undergraduate research in chemistry and biology at an R1 institution. **J.A. Greenberg**

11:00 310. Context-based learning: Teaching green chemistry through soy-based innovations. **M. Hensley**, J.E. Wissinger, M.T. Wentzel, K. Weigal, R. Heggs, o. villanueva, A.S. Cannon

11:20 Panel discussion - 10 minutes.

Coatings and Surface Chemistry

Alvarado Salon DE

Cosponsored by COLL
D. J. Rodriguez, *Organizer, Presiding*

9:00 Introductory remarks.

9:05 311. Smart hydrogel coatings enable iron-responsive drug release for mitigating neural implant rejection. **J. Maleszka**, E. Attah, I. Tsironi, M. Franklin, A. Prasad, J. Olivier

9:25 312. Thick uniform coatings on hollow glass microspheres via DC magnetron sputtering. **K. Shulman**, D. Ross, D.J. Rodriguez, V. Siller

9:45 313. Molten metal interaction with metal oxide surfaces. **D.J. Rodriguez**, K. Shulman, M. Oltmanns, D. Ross, V. Siller, B. Morrow

10:05 Break.

10:20 314. Process optimization of molten salt electrodeposition for refractory metal coatings. **O.R. Dale**, N. Rood, M.J. Monreal, J. Chamberlain

10:40 315. Electrodeposition of manganese as a surface coating for enhancing pulsed power physics at Sandia's Z-machine. **T.S. Watkins**, V. Gayoso, M. Stalcup, A. Sarracino, D. Lamppa

11:00 Break.

11:15 316. Effect of ligand substitution for zirconium carbide chemical vapor deposition (CVD). **M. Christian**, S. Goodman-Miller, J. Bossiere, H. Root

11:35 317. Promotion of epoxy/ceramic interfacial adhesion through chemical vapor deposition of silane coatings. **A. Grife**, J. Dugger, E.C. Larkin, J. Quinn, J. Duay, S. House, R. Goeke, L. Takahashi, M. Pham

Name	Paper Number
AKRAM, M.	154, 156, 157, 205
Abadam, C.	298
Abebe, W.	117
Acharya, B.	241
Addamane, K.	249
Addison, B.M.	269
Adekoya, S.B.	146
Adesunloye, T.	87
Adhikari, A.	259
Adolphi, N.	43
Agblevor, F.A.	90, 300
Ager, J.	10
Ahangari, M.	62
Ahn, J.	11
Akinlabi, B.	288
Al-Obeidi, F.A.	22
Alcantar-Velasquez, E.	295
Alfaro, B.	133
Ali, A.	187, 292, 295
Alwis, D.	155
Anderson, M.J.	41
Anderson, R.G.	273
Andersson, A.	27, 29
Anderton, C.R.	214
Andrews, M.	156
Anjum, R.	279
Antoninka, A.	96
Apawu, A.K.	132
Apodaca-Sparks, A.	187, 298
Appelhans, L.	2
Archer, S.	112
Armijo, Z.E.	104
Astle, S.	38, 68
Atchley, C.	298
Atlas, S.R.	5, 189, 208, 210
Attah, E.	311
Atteberry, M.	152
B. Cox, M.	175
Babuska, T.F.	219
Banerjee, A.	26
Barache, Y.	72
Barela, L.	43, 115
Barrett, N.	3
Barros, K.	177
Bartholomeusz, J.A.	98
Baten, A.J.	71

skandarajan, M.	37
villanueva, o.	310
wang, y.	195