### Session A: Genomics & Computational Biophysics (Luminaria)

### **Fine-Tuning Large Language Models for Genomic Intelligence** Huixin Zhan, NMT

The intersection of artificial intelligence and genomics is transforming our ability to decode the functional impacts of genetic variations, yet several computational challenges persist, including scalability, disease specificity, and adaptability to heterogeneous genomic data. This presentation introduces two AI-driven frameworks, DYNA and LINGO, which leverage machine learning and natural language processing (NLP) innovations to address these limitations in genomic analysis. DYNA leverages a Siamese neural network to fine-tune genomic foundation models for precise, disease-specific predictions, treating the genome as a structured language where genetic variants function like syntax or grammar rules. It adapts pre-trained embeddings to domain-specific tasks, achieving state-of-the-art performance in variant effect prediction and generalizing to unseen variants. This demonstrates how task-specific fine-tuning transforms pre-trained models for specialized biomedical challenges, similar to NLP applications like semantic similarity or translation. LINGO reimagines genomic data processing by extending NLP foundation models to genomic sequences. Leveraging a novel prefix-based tokenization strategy and adaptive rank sampling for parameter-efficient fine-tuning, LINGO achieves unparalleled scalability and performance across genome annotation tasks. Together, DYNA and LINGO illustrate how AI and machine learning methodologies can redefine computational genomics. These frameworks offer a glimpse into the future of AI as a transformative tool in biomedicine, bridging machine learning with precision genomics.

#### **Replication Across the Alkylated DNA Lesions**

Myong-Chul Koag, ENMU

DNA is continuously insulted by a wide range of endogenous and exogenous alkylating agents to generate various alkylation lesions, which can interfere with DNA replication, transcription and genomic integrity. Among them, N7-methylguaine (7MeG), O6-methylguanine (6MeG), and N3-methyladenine (3MeA) are three major methylation adducts, which account for up to 90% of the total alkylation lesions in DNA. High-resolution of crystallographic structures and steady-state kinetics from our research team have provided structural and mechanistic insights on how 7MeG and 6MeG lesions are replicated by human DNA polymerase  $\beta$ , a valuable model of replicative polymerase for studying the effects of DNA lesions on replication efficiency and fidelity of DNA polymerase. However, the atomic resolution structure of DNA polymerase replicating 3MeA has not been reported yet, even though several reports on the reduced catalytic efficiency and fidelity with a few polymerases have been published. The 3MeA is known to be highly cytotoxic, because it generates a steric bulk on the minor groove of DNA and hinders DNA polymerases. In this talk, recent progress and implications on how the minor groove lesions have effects on kinetics and function of DNA polymerases will be presented.

### Session A: Genomics & Computational Biophysics (Luminaria)

#### Role of Dietary Flavonoids in r(CAG) RNA Repeat Expansions Diseases Nabanita Saikia, NMHU

Huntington's disease (HD) is a rare polyglutamine neurodegenerative disorder, caused by the aberrant genomic expansion of cytosine-adenine-guanine trinucleotide repeats (CAG)n in the first exon of the huntingtin gene. Repeat lengths beyond the pathogenic threshold of 36 lead to protein misfolding, aggregation, cellular dysfunction, and progressive neurodegeneration. Although the precise mechanisms of repeat expansion and HD pathogenesis remain unclear, studies suggest that slipped DNA and RNA intermediates stabilized by A·A mismatches contribute to toxicity through the formation of extended hairpin structures. The study aims to investigate the therapeutic potential of dietary flavonoids, naturally occurring polyphenolic compounds with known antioxidant and neuroprotective properties, as small-molecule inhibitors that selectively bind to A·A mismatches in (CAG)n hairpin structures. The central hypothesis is that certain flavonoids can destabilize toxic secondary structures by binding selectively to A·A mismatches through hydrogen bonding,  $\pi$ -stacking, and/or base intercalation. The research aims to investigate the structure-activity-property relationship of flavonoids and predict flavonoid binding to (CAG)n repeats. Unlike prior studies that focused solely on protein aggregates, this research will challenge the prevailing protein-centric paradigm, by specifically targeting pathogenic (CAG)n DNA/RNA intermediates, central to repeat expansion disorders. The goal is to contribute to the development of RNA-targeted therapeutics using smallmolecule inhibitors that address the underlying molecular etiology of HD and related neurodegenerative diseases.

### Session B: New Mexico Space Grant Fellows (Santa Ana B)

Constraining Mineralogy of Martian Analog Sulfates From the Quebradas Area, New Mexico Luc Carbonneau, NMT

Situated only a few miles east of Socorro is a vast desert landscape known as the Quebradas. The Quebradas contain Paleozoic evaporite deposits, including massive gypsum in the Yeso and Atrasado Formations. Due to the presence of this sulfate mineral and the accessibility of the location, the Quebradas offer a unique setting for studying minerals that could serve as Martian analogs. In September of 2023, teams from NASA's Goddard Space Flight Center (GSFC) and Johnson Space Center sampled gypsum from the Yeso Formation to test its viability as a depositional analog for sulfates found on Mars. During an internship at GSFC over the summer of 2024, initial analyses of mineralogy and organic content were performed. While small amounts of carbon were detected in some samples, it was not immediately clear whether this carbon was from an organic or mineral source. We suspect that carbon found in Quebradas gypsum is likely from mineral sources rather than preserved organics, but that organic carbon would be found in higher abundance in associated clays. If this hypothesis is correct, sulfates may not be suitable targets for assessing organic preservation on Mars, and different target formations or a new approach for detecting organic molecules would be needed. To better constrain the mineralogy and organic carbon content of sulfate minerals in the Quebradas, samples from the Upper Yeso Formation (Permian), Atrasado Formation (Pennsylvanian), and more recent lacustrine deposits from the central Rio Grande rift (Miocene) were collected for further analysis. To constrain the mineralogy and depositional environment of these samples, we performed powder X-ray diffraction (pXRD) and petrography of thin sections. Organic preservation will be determined by infrared spectrophotometry. pXRD analyses of Quebradas samples found minor calcite, while similar analyses of Miocene lacustrine samples found no carbon-containing minerals. Calcite was not observed in thin section, either because of the size of the grains or the abundance in the sample. This result indicates that the carbon content of Quebradas samples collected in 2023 by teams from NASA may be influenced by mineral sources rather than residual organics.  $\delta$ 34S values of the Paleozoic sulfates range from +12.6 to +17.6%, while  $\delta$ 34S values of the Miocene sulfates range from +3.8 to +6.5%, showing values overall consistent with an evaporitic depositional environment, although with some variability that could be due to differences in specific depositional or diagenetic conditions. Although it seems likely that the bulk sulfates have very little, if any, preserved organics, ongoing analyses will continue to explore other sulfate-associated minerals and evaluate spatial associations among geochemical, mineralogical, and depositional signatures in the older and younger sulfates.

This research is based upon work supported by the New Mexico Space Grant Consortium (NMSGC) Space Grant Fellowship through a NASA Cooperative Agreement No. NM-80NSSC25M7069.

### Session B: New Mexico Space Grant Fellows (Santa Ana B)

### Gravitational Instability in the AB Aurigae system: Investigating the Pebble Ring Via 2D Simulations

Eleanor Serviss, NMSU

Giant planet formation remains an open question: how do planets that are multiple times the mass of Jupiter form far out in planetary systems where temperatures are cooler and densities are lower? There are two main proposed formation pathways: core accretion and gravitational instability. Core accretion is a bottom-up method where a rocky core forms from smaller bodies before accreting a gaseous envelope. Planets like Jupiter may have formed through accretion. Gravitational instability, however, is a top-down method where material clumps together when self-gravity overbalances the resisting pressure and shear forces. This is how stars form, and it may be a formation pathway for brown dwarves and multi-Jupiter mass planets. Although numerical models reproduce gravitational instability forming planets in disks, so far, the most convincing observational evidence for a planet that formed via gravitational instability is AB Aurigae b (Currie et al. 2022). This project focuses on the AB Aurigae system and is a follow-up of the modeling done in Currie et al. (2022), this time to reproduce a pebble ring feature seen in the AB Aurigae disk beyond the potential gravitational-instability formed protoplanet.

In this talk, we use a 2D shearing box simulation, which approximates the protoplanetary disk as a locally linear square box. We test how the Toomre instability parameter parameter (Toomre Q), which measures the ratio of compressive versus shear and expansive forces, varies over time. We use a cosine-wave density profile and pressure equilibrium to create a Toomre-Q profile that is initially unstable in the center (Q<1) and stable on the inner and outer edges of the box. We observe that the shearing box initially becomes more unstable in the center before shocking and heating up. We investigate whether there is Rossby Wave Instability in the transition between Q stable and unstable. This provides the foundation for further work that will see if the AB Aurigae pebble ring is reproduced on this boundary. In this transition zone, we predict there will be a concentration of gas and mass that creates a pressure bump. This pressure bump could, in turn, trap pebbles and form a pebble belt, like the one seen in AB Aurigae.

This research is based upon work supported by the New Mexico Space Grant Consortium (NMSGC) Space Grant Fellowship through a NASA Cooperative Agreement No. NM-80NSSC25M7069.

# **Shock-wave Boundary Layer Interactions in Collaborative Combat Aircraft Formations**Darrien Williams, NMT

The future of U.S. air supremacy hinges on sixth-generation fighter aircraft which will coordinate with semi-autonomous drones flying in formations at supersonic speeds. These formations impact radar detectability, payload delivery, and fuel efficiency, with shock wave boundary layer interactions (SWBI) playing a key role in determining viable configurations. This study examines SWBI between aircraft operating at Mach 2 using ANSYS FLUENT, focusing on

### Session B: New Mexico Space Grant Fellows (Santa Ana B)

pressure, temperature, and Mach number differences between leading and trailing aircraft. Results show that a trailing aircraft positioned within a shock wave experienced a 108% increase in upper surface pressure and a 35% decrease in lower surface pressure. Increasing the leading-edge distance to position the trailing aircraft within expansion waves, upper surface pressure increase was reduced to 62.6%, while the lower surface pressure decrease was reduced to 12.4%. These pressure differentials can disrupt control and lift surfaces, decrease fuel efficiency, and compromise mission success. Optimizing formation development based on mission requirements will help minimize radar cross-section, increase fuel efficiency, and ensure successful payload delivery. As the development of the high-speed aircraft utilized by sixth generation fighters continues, understanding the SWBI effects in formation becomes crucial for mission success.

This research is based upon work supported by the National Aeronautics and Space Administration under NASA Cooperative Agreement No. 80NSSC20M0034 through the New Mexico Space Grant Consortium.

### **Zinc Electrodeposition Under Varying Gravitational Fields for Advanced Batteries**Ngoc Nguyen, UNM

Understanding how gravity influences zinc electrodeposition is essential for optimizing zincbased batteries for grid storage on Earth and for power systems operated in altered-gravity environments. Here, we experimentally probe the coupling between gravitational forces and interfacial growth by manipulating the orientation of the electric field relative to gravity during zinc plating/stripping in an aqueous ZnSO<sub>4</sub> electrolyte. Two configurations were examined: "under-gravity," in which the electric field is aligned with gravity, and "against-gravity," in which it is oriented oppositely. By reversing the anode/cathode positions while keeping all other operating parameters constant, we aimed to understand the gravitational effects on the nucleation and mass transfer in the system. The analysis integrates classical nucleation and growth concepts with hydrodynamic flow considerations to interpret differences in morphology and electrochemical behavior. Scanning electron microscopy reveals that the against-gravity orientation promotes uniform, layer-like zinc growth with reduced lumps, suggested homogeneous ion flux at the interface. Correspondingly, the against-gravity configuration exhibits a more stable voltage profile during charging, indicating mitigated concentration polarization and improved interfacial stability. Taken together, these results suggest that controlling cell orientation—therefore the direction of buoyancy-driven convection and particle/ion transport—be an effective, regulate zinc growth uniformity and crystal texture. The insights provide a framework for designing zinc anodes with improved reliability and safety across terrestrial and space-relevant conditions, and they highlight orientation as a practical parameter for future studies in altered-gravity electrochemistry.

This research is based upon work supported by the New Mexico Space Grant Consortium (NMSGC) Space Grant Fellowship through a NASA Cooperative Agreement No. NM-80NSSC25M7069.

### Session C: Environmental Engineering & Economics (Santa Ana A)

### Which Sources are Contributing? A Source Characterization of VOC Concentrations Outdoors in Albuquerque, New Mexico

Jaimie Ritchie, UNM

The prevalence of VOCs from manufacturing and other sources is increasing as industry develops, leading to higher exposure in industrial and environmental justice (EJ) communities, such as the South Valley of Albuquerque, a low-income, Hispanic region. In response to the community's air quality concerns, the City of Albuquerque began measuring Volatile Organic Compounds (VOCs) but has not reported the results due to data processing challenges.

Many VOCs have adverse health impacts due to carcinogenicity and respiratory repercussions, but no ambient air regulations exist. The quantity of VOCs adds to the complexity of analysis, which can be simplified through source characterization. This project will conduct high quality data analysis with community input and communicate the results to the community to help them understand their air pollution.

We hypothesize that VOCs from similar sources (industrial, construction, motor exhaust, etc.) will have similar trends in peaks and frequencies. We are conducting a variability analysis of 124 VOCs measured by GC-FID in the South Valley. We are performing source characterization of VOCs utilizing Positive Matrix Factorization (PMF), the results of which are being used to assess temporal variability of sources and analyze wind direction tendencies.

This analysis will illuminate what emission sources may be contributing to air pollution in the South Valley and facilitate interpretation of future values measured at the site. The results will inform the community what is in their air, and the assessment process can be shared with communities elsewhere who are facing similar challenges.

# Dynamic Optimization of Nuclear Power Plant Retirement Timing: The Case of Diablo Canyon, California

Refat Mishuk, UNM

The Nuclear Regulatory Commission authorized two different decommissioning methods for nuclear power plants: "DECON" (Decontamination) and "SAFSTOR" (Safe Storage). After the retirement of the nuclear power plant, radioactive materials and equipment are dismantled under DECON. In contrast, the power plant is left intact for a period to allow radioactive materials to decay before dismantling under SAFSTOR. DECON is the faster decommissioning method, typically completed within 10 years. Whereas SAFSTOR allows for deferred dismantling with a containment period up to 50 years. The study developed a dynamic optimization model to assess the optimal retirement time of the Nuclear Power plants based on decommissioning methods. The model was applied to the Diablo Canyon nuclear power plant (DCPP), which has been providing electricity since 1985 in California. The power plant was initially planned to retire in 2024-25 and scheduled for DECON decommissioning. However, the operation of the power plant has been extended for an additional 5 years. The study found out optimal

### Session C: Environmental Engineering & Economics (Santa Ana A)

shutdown time of DCPP varies from 35.07 to 56.29 years (for 5% to 7% discount rate) for DECON. For SAFSTOR, the study found an optimal shutdown time of 35.81 to 65.46 years (for 2% to 4% discount rate). The result suggested that DECON may no longer be an economically effective decommissioning strategy for DCPP, considering the five-year extension and a low discount rate.

#### What are Carbon Credit Markets and How Do They Work?

Clinton Owusu, NMSU

Several initiatives allow farmers and ranchers to generate additional income by adopting management practices that store carbon in soil through carbon credits. A carbon credit is traded globally for greenhouse gas emissions reductions caused by implementing management practices and is expected to be purchased by entities and corporations to meet their climate change goals.

In the United States, carbon markets are voluntary, and until today, there is no universal price for the carbon stored on agricultural lands, which implies that prices are primarily driven by supply and demand, like other commodities. However, the current agricultural carbon credits market is not mature and difficult to characterize as the available carbon credit programs have different rules, incentives, and penalties (Plastina 2021). This paper aims to help farmers, ranchers and Extension professionals, interested in carbon credit programs better understand how carbon credit and carbon trading work in the U.S. It provides information on the market's mechanisms, specificities, and available carbon programs in the U.S.

### Measuring Consumptive GPCD in the ABCWUA Service Area

Stephania Alarcon, UNM

Every few decades, scholars have revisited how water is used and valued in the Middle Rio Grande Valley (MRGV). Earlier assessments coincided with major shifts, such as the construction of the Middle Rio Grande Conservancy District in the 1930s (Cockerill and Walker, 1931), the introduction of San Juan,ÄìChama Project water in the 1960s (Wolman et al., 1962), and recognition of groundwater limits in the 1990s (Brown et al., 1996). Roughly thirty years have now passed since those studies, and new pressures such as climate change, continued population growth, municipal conservation gains, contraction of commercial agriculture, and endangered species requirements again raise questions about the value of water in competing uses. Information that links water use to community values can provide a stronger basis for public dialogue about future conditions in the MRGV. Cities in arid regions need measures that reflect how much water is actually used, not just withdrawn.

In Albuquerque's MRGV, the common metric (Gallons per Capita per Day (GPCD)) tracks total diversions to the municipal system and can overstate pressure on supplies because a large share of that water returns to the river as treated effluent. I define and implement

### Session C: Environmental Engineering & Economics (Santa Ana A)

Consumptive Gallons per Capita per Day (CGPCD), which subtracts measured return flows from total diversions, to better represent water that is evaporated, transpired, incorporated into products, or otherwise unavailable locally.

Using monthly data (2015-2024) reported by the Albuquerque Bernalillo County Water Utility Authority (ABCWUA), including diversions, return flows, and a population series based on active service connections and Census household size, I compute GPCD and CGPCD at monthly and annual scales. I then compare levels, variability, and seasonal patterns to assess how much insight is lost when relying on diversion-based GPCD alone.

Results show a large, policy-relevant gap: average GPCD = 128.95 gallons/person/day while average CGPCD = 54.51, implying that only 42% of diverted water is consumptively used on average (58% returns to the system). Variability differs sharply: coefficients of variation are 0.31 for GPCD versus 0.70 for CGPCD, indicating that consumptive use is far more seasonal and volatile, consistent with outdoor irrigation and weather. The CGPCD range (about -3.6 to 142.2) highlights months with very low net consumption and occasional measurement noise; GPCD ranges from 76 to 229. These patterns persist across years, even as conservation policies and population change.

CGPCD provides a clearer signal of resource pressure than diversion-based GPCD and better supports decisions about conservation targets, rate design, seasonal watering rules, and tradeoffs among municipal greenness, heat mitigation, and instream ecological needs. Because CGPCD ties directly to consumption, it aligns more closely with sustainability and fairness discussions, how much water residents truly use, when they use it, and what benefits those uses create. This municipal CGPCD framework can be paired with remote-sensing estimates for agriculture to compare consumptive use across sectors and to inform future allocation debates as climate warming tightens hydrologic budgets.

### **Session D: Engineering** (Acoma B)

### Development of New Mexico STEM Workforce through Additive Manufacturing Integration in K-12 Education

Rigesh Krishnaraj, NMSU

Additive Manufacturing (AM) or 3D printing is a process of making three-dimensional objects from digital models. STEM (Science, Technology, Engineering, and Mathematics) as an interdisciplinary approach to teaching and learning prepares students with skills and competencies essential for today's workforce. 3D printing in K-12 classrooms can advance STEM learning and prepare students for STEM careers. The research question was: How does the DREAM (Distributed Resilient and Emergent-intelligence-based Additive Manufacturing) professional development (PD) in AM for K-12 teachers in New Mexico influence their perceptions of the relevance of AM in K-12 education? A qualitative approach was used to collect and analyze data from surveys and focus group discussions from ten participants. We found that prior to the PD, 90% of participants reported no familiarity with AM and lacked knowledge of how to integrate it into their teaching. Post PD, all participants expressed their familiarity with AM and enhanced confidence and motivation to integrate AM in teaching and learning. Eight teachers are currently teaching AM in K-12 classrooms. The reasons for teachers' shift in perception and motivation to integrate AM in their teaching were, 1) teaching abstract concepts through hands-on practices enhances engagement, interaction, and deepens conceptual understanding; 2) recognizing AM's connection to STEM careers, teachers emphasized that developing 3D printing skills can spark interest in engineering, design, and innovation, preparing students for future careers. Equipping teachers with the skills and resources for teaching AM will strengthen STEM instruction and will support future workforce development in NM.

### Remediation of Uranium from Water Using a Water-insoluble Organic Compound Water Purification

Matthew Ogbe, ENMU

Groundwater is the most important source of freshwater for drinking, irrigation and dairy production. The wide occurrence of dissolved uranium in groundwater is of increasing concern to human health and ecological safety throughout the world because of its radioactivity and chemical toxicity. Uranium is introduced into groundwater by a number of natural geochemical processes including the dissolution of minerals, release of adsorbed uranium by desorption from minerals and rocks, as well as by human activities that include uranium mining for nuclear fuel and the treatment of phosphate rocks as fertilizers. The combined effects of the abovementioned sources lead to the contamination of groundwaters which is a global environmental problem of critical concern to agricultural ecosystems and public health. It is, therefore, of vital importance to develop a practical and sustainable method to remediate uranium from contaminated groundwater. The established approaches of uranium remediation such as adsorption, photocatalysis, electrocoagulation, ion exchange and membrane filtration have the common drawbacks of being too expensive and technically unsuitable for large-scale remediation, especially in real waters that contain various mineral ions and other organic and

### **Session D: Engineering** (Acoma B)

inorganic constituents. The design of a simple, low-cost, and high-efficient uranium remediation process from contaminated water is of great necessity in order to protect our drinking water and maintain agricultural and dairy production. In the current study, a synthesized water insoluble organic ligand was used to remediate uranium from a laboratory prepared uranium(II) acetate solution. The ligand was prepared by refluxing a mixture of terephthaldehyde and Lcysteine in methanol for 24 hours, followed by filtration, washing with methanol and distill water and air-drying. The prepared ligand was then employed to remediate a 0.0122M, 0.022M and 0.032 M uranium acetate solution at various doses (0.05-0.20 g). The absorption efficiency of the ligand for uranium was found to be moderate and increased with an increase in the ligand dose from 10% at 0.05g to 38% at 0.20g for the highest prepared concentration (0.032M uranyl acetate). The ligand that was pre-treated by 0.05 M KOH, however, showed improved absorption efficiency, giving 53% and 71% for 0.05 and 0.20 g respectively. This increase in the uranium removal efficiency by the ligand might be due to an increase in the available binding sites or a change in the surface charge characteristics of the ligand due to the KOH treatment or the deprotonation of the carboxylic group to carboxylate anion (of the ligand). The results of this study suggest that low cost chemically modified ligands are a good candidate as a functional material for the remediation of uranium from groundwater. Additionally, the ligand produced an excellent extraction efficiency when the concentration of the uranyl acetate was lowered (at 0.012M and 0.022M).

### The Removal of Abiotic Ash from Algal Biomass for Sustainable Development of High Value Carbon Materials

Elijah Asamoah-Amoateng, ENMU

The increasing demand for sustainable and high-performance materials has led to significant interest in the development of carbon-based materials derived from renewable sources such as algal biomass. Algae, due to their high carbon and lipid content, fast growth rates, and minimal land use, are considered a promising feedstock for bio-based carbon materials. However, the presence of abiotic ash (inorganic elements such as metals and minerals) in algal biomass hinders the efficient conversion of algae into high-value carbon materials. This work focuses on various methods for the efficient removal of abiotic ash from algal biomass, analyze their impact on the properties of the derived carbon materials, and propose a sustainable pathway for the development of high-value carbon products. The ultimate goal is to contribute to the creation of a circular economy by using algal biomass for the production of high-performance carbon materials with applications in energy storage, water purification, and catalysis.

### **Uncertainty-Aware Deep Reinforcement Learning for Robust Autonomous Voltage Control** Seyi Fanifosi, NMSU

Deep reinforcement learning (DRL) has advanced autonomous voltage control (AVC) in modern power systems by addressing complex operational challenges. However, the black-box nature of DRL raises concerns about reliability, especially under uncertainty. Aleatoric uncertainty,

### **Session D: Engineering** (Acoma B)

from inherent system randomness, and epistemic uncertainty, from limited knowledge, can lead to suboptimal control actions and threaten voltage stability. Existing DRL-based AVC methods largely ignore these uncertainties, restricting their real-world applicability. This paper proposes an uncertainty-aware DRL framework that integrates an ensemble quantile network (EQN) into a deep deterministic policy gradient (DDPG) agent. The framework estimates both aleatoric and epistemic uncertainties in real time and dynamically refines actions through uncertainty-aware quadratic optimization. Case studies on a large-scale power system show that the proposed approach improves robustness, maintains voltage regulation under out-of-distribution conditions, and reduces the number of iterations required for stabilization compared to conventional DRL agents.

### **Session E: Advanced Materials for Energy Applications** (Acoma A)

### Carbonyl-Functionalized Penta(p-Phenylene): Synthesis and Characterization Organic Synthesis

Isaac Ahinful, ENMU

One way to convert light into electricity is through organic solar cells, which employ conductive polymers or tiny organic molecules. In response to the growing need for sustainable power, solar cell research and development, production, and distribution have all experienced meteoric rises in the last two decades. Research into electron delocalization in organic semiconductor capacitors (OSCs) requires the synthesis of carbonyl-functionalized penta-(p-phenylene). This procedure includes adding an infrared reporter (a carbonyl group) to the penta-(p-phenylene) backbone. Following time-resolved infrared investigations of electron delocalization, pulse radiolysis follows. This approach has the potential to revolutionize several disciplines by revealing and manipulating the electrical characteristics of different materials. Organic electronics, photovoltaics, and molecular electronics are just a few examples.

# Comparison of catalytic reduction of carbon dioxide between Manganese and Ruthenium complexes of a pyridine-based polyamine macrocycle

Md Mhahabubur Rhaman, ENMU\*; Dr. Eric S. Wiedner, PNNL

Over the last two decades, numerous catalysts, comprising a diverse array of metals and ligands, have been reported for hydrogenating CO2 to produce high-energy-density chemicals. However, their kinetics, efficiency, solvent, stability, and expense must still be suitable for large-scale and economical energy processes. Therefore, new approaches and detailed mechanistic catalysis studies are in demand, utilizing cheap, readily available, and environmentally friendly chemicals. In this proposal, phosphene-free, a pyridine-based polyamine macrocycle was synthesized from commercially available compounds and converted to Mn(I) and Ru(II) complexes by reacting with commercially available [Mn(CO)5]Br and Ru(DMSO)2Cl2 in refluxing methanol. The abilities of these complexes to catalytically hydrogenate carbon dioxide were studied using an organic base, DBU (1,8diazabicyclo[5.4.0]undec-7-ene), at 500 psi of a 1:1 ratio of H2 to CO2 at 80 C in acetonitrile solvent in a batch reactor. Under these conditions, both complexes exhibited catalytic activity with various turnover numbers (TONs) for formic acid. Since, without a base, the complexes didn't show catalysis, suggesting a key role of DBU in activating the complexes for catalysis. Various ratios of DBU with the catalyst were used to determine the role of DBU in the hydrogenation process. Although the Mn(I) complex exhibited a lower TON of formic acid compared to the Ru(II) complex, Mn is inexpensive, readily available, and biocompatible. Both complexes are air and moisture-stable. Acknowledgment: Assistant Prof. Md Mhahabubur Rhaman was supported by the U.S. Department of Energy, Office of Science, Office of Workforce Development for Teachers and Scientists (WDTS) under the Visiting Faculty Program (VFP). Dr. Eric S. Wiedner was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division, Catalysis Science program, FWP 47319.

### **Session E: Advanced Materials for Energy Applications** (Acoma A)

# Electrochemical studies of pentacyanodimethylsulfoxide ferrate(II) and tetracyanobisdimethylsulfoxide ferrate(II): A novel example of sulfoxide isomerization on iron(II)

Seyi Adekoya, CNM

The reversible isomerization of sulfoxide ligands in transition metal complexes has been extensively documented in Ru(II) chemistry, yet remains unexplored in Fe(II) systems. This research addresses that gap by investigating sulfoxide linkage isomerization in pentacyano- and tetracyano-bis(dimethylsulfoxide) ferrate(II) complexes, with the aim of understanding their redox behavior, electronic structure, and potential for photonic applications. The hypothesis is that sulfoxide ligands undergo S->O and O->S isomerization upon oxidation and reduction, respectively, and that this transformation is influenced by solvent environment and ligand substitution. Fe(II) sulfoxide complexes were synthesized and characterized using <sup>1</sup>H NMR, IR, and UV-vis spectroscopy. Electrochemical studies were conducted in various solvents using cyclic voltammetry, and isomerization kinetics were evaluated using Nicholson-Shain analysis. Results reveal solvent-dependent isomerization and measurable shifts in reduction potentials, confirming reversible linkage isomerization. Notably, spectroelectrochemical studies demonstrated the formation of O-bonded isomers post-oxidation, with distinct spectroscopic signatures. Furthermore, substitution of methyl groups with bulkier ligands altered redox potentials and absorption maxima, indicating electronic tunability. Comparative studies with Ru(II) analogs showed linear trends in reduction potential, suggesting Fe(II) as a cost-effective alternative for light-driven applications. This study establishes the first example of sulfoxide isomerization in Fe(II) and contributes foundational knowledge for the development of ironbased photochromic and photoredox systems. The findings are significant for advancing sustainable technologies in solar energy conversion, data storage, and molecular switching.

### Ligand Tuning for Stabilization of <sup>3</sup>MLCT States in Fe(II) Complexes for Solar and Photonic Applications

Seyi Adekoya, CNM

The stabilization of the triplet metal-to-ligand charge transfer ( ${}^{3}$ MLCT) state in Fe(II) complexes has attracted significant interest due to its potential in solar energy conversion, photoswitches, photoresponsive materials, and photocatalysis. This project investigates the mechanisms underlying  ${}^{3}$ MLCT stabilization by synthesizing a series of  $[Fe(CN)_5(L)]^{3-}$  complexes, where L includes pyridine, quinoline, isoquinoline, and their derivatives. Variable-temperature NMR and electrochemical analyses were carried out across multiple solvents, revealing solvent interaction with the cyanide ligands. Transient absorption spectroscopy will probe the excited-state dynamics to further elucidate relaxation pathways and excited lifetime. By clarifying the electronic interactions that govern  ${}^{3}$ MLCT behavior, this research aims to optimize the stability and efficiency of iron-based charge transfer states, contributing to the design of advanced photonic and catalytic materials from earth-abundant iron complexes.

### Session F: Biology (Isleta)

### From Invasive Weed to a Resource: Evaluating Salsola tragus Potential through Undergraduate Research

Audrey Lee, UNM

Salsola tragus, commonly known as Russian thistle, is an invasive species in North America but has been traditionally used in Middle Eastern medicine for its antibacterial, antifungal, and anti-inflammatory properties. Despite its global distribution, research in North America has focused mainly on its ecological impact, leaving its bioactive potential largely unexplored.

This study addresses that gap by evaluating extraction methods to isolate essential oils and organic compounds for further analysis from Salsola tragus. Four solvent-based techniques were tested: ethanol Soxhlet extraction, ethanol-based solvent extraction, acetone, and isopropanol, alongside hydrodistillation and microwave-assisted extraction. Ethanol Soxhlet extraction had the highest yield at 2.9%, compared to 2.2% for ethanol solvent extraction. Water-based and microwave-assisted methods were found to be ineffective due to contamination and low extraction performance.

Literature indicates that the species shows high genotype diversity and complex hybridization, which may contribute to regional variation in chemical composition. These findings support future work in compound identification using mass spectrometry and bioactivity testing through in vitro assays to validate medicinal potential and compare regional chemical differences between North American and Middle Eastern populations.

This undergraduate-led project also highlights how research with local plants can enhance STEM education. By using accessible materials and low-cost methods, the project shows that undergraduates can engage in meaningful chemical research. Integrating local flora into the curriculum promotes hands-on learning, increases engagement, and demonstrates that chemistry is not confined to labs but is part of the world around students, making science more inclusive and relevant.

### Studying Conservation Genetics with the Turner Aquatic Conservation Lab Internship Rachel Mann and Renee Pena, UNM

The Turner Lab at the University of New Mexico studies the genetics of fish species native to semi-arid regions of the American Southwest to better understand how genetic diversity changes over time. During this internship, work focused primarily on the endangered Rio Grande silvery minnow (Hybognathus amarus) and the critically endangered Bonytail (Gila elegans). The Rio Grande silvery minnow inhabits a 280 km section of the Rio Grande River, and long-term genetic monitoring allows investigation of how early life-history features and supportive breeding influence its genetic characteristics. Using modeling and genetic analysis, the lab studies how demography, environmental change, and management actions affect diversity across time and space. For the Bonytail, which suffers from a severe genetic bottleneck, genetic sequencing is used to examine parentage and reproductive ecology in

### Session F: Biology (Isleta)

hatchery populations. Laboratory work included DNA isolation from fin clippings, PCR amplification, gel electrophoresis, DNA quantification using a Nanodrop, BigDye sequencing reactions, and GT-Seq (Genotyping-in-Thousands by sequencing) cleanups. These methods allow efficient analysis of genetic diversity and structure among fish populations. The internship provided experience in molecular biology techniques, sterile laboratory practice, and data analysis relevant to conservation genetics. This work contributes to understanding the genetic effects of captive breeding and environmental stress on endangered freshwater fish species.

#### **West Nile Virus Dynamics in Southwestern Culex Populations**

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Mosquito-borne diseases remain a persistent and expanding threat to public health. In the United States, West Nile virus (WNV), transmitted primarily by Culex mosquitoes, continues to cause severe neurological illness and recurrent seasonal outbreaks. As of October 14, 2025, 1,564 human WNV cases have been reported nationally, including 26 in New Mexico. In this study, Culex quinquefasciatus and Cx. tarsalis were analyzed from 23 surveillance sites along the Rio Grande Bosque between 2023 and 2025 to determine WNV infection rates and temporal patterns. Mosquitoes were pooled (5,Äì50 insects) by date, site, and species, and screened by RT-qPCR for WNV RNA. Weekly totals of mosquitoes, WNV-positive pools, and minimum infection rates (MIRs) were calculated. Across the three-year period, 8,881 Culex quinquefasciatus and 8,587 Cx. tarsalis were processed, forming 527 and 417 pools, respectively. WNV-positive pools numbered 90 (21.2%) in 2023, 18 (24.8%) in 2024, and 105 (20.5%) in 2025, yielding mean MIRs of 12.8, 11.4, and 12.5 per 1,000 mosquitoes, respectively. Temporal analysis showed peak abundance and infection from mid-July to mid-August, coinciding with optimal breeding temperatures and the migratory activity of avian hosts, which likely amplifies local viral transmission. These results demonstrate consistent WNV circulation within the Rio Grande corridor and underscore the importance of sustained entomological surveillance, spatial-temporal modeling, and integration of climatic and ecological data to forecast arboviral risk. Continuous monitoring will be critical to guide targeted vector control and to mitigate future WNV outbreaks in New Mexico and the broader southwestern United States.

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#### **Mosquito Trapping with Various Odorants**

Amelia Witney, UNM

This study aims to explore the efficacy of a mosquito trap, baited with different human and animal biological materials, in attracting various mosquito species, with a focus on the distribution of species, prey populations, and regional viral diversity and impact. While extensive research exists on trap techniques and human-odor attractants, research on non-human biological material-based traps is limited. Expanding that research would address the critical role of mosquitoes as vectors for reservoir-host-dependent viruses, like West Nile Virus (WNV).

Our research will not only assess the relationship between trap success and odor baiting but also species-specific odor preferences, allowing us to quantify how likely different mosquito species are to infect humans with a vector-borne illness. Future projects will involve qRT-PCR to determine the origin of mosquito blood meals and to develop assays for viruses prevalent in the southwestern United States.

Our research will be conducted at multiple locations in central and northern New Mexico, and will utilize low-cost trap designs. Five traps will be deployed at each site, following a Latin square protocol, with one control lacking odorant. Samples will be collected every 24 hours, over a five-day period, and then sexed, speciated, and stored at -80C for future research.

The importance of this research lies in its potential to aid in the development of a low-cost, species-targeted, high-impact surveillance method suitable for rural areas with limited healthcare resources. Our results will guide future research targeting the relationship between mosquito species and the transmission of arboviruses to human hosts.