Second Annual State Conference
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New Mexico State University
Poster Presentations
Abstracts

Eastern New Mexico University

Emmanuel Amoah
Graduate Student
Physical Sciences/Chemistry

"Electrochemical Biosensor Arrays Based On Viologen-Functionalized Monolayers"
Authors: Emmanuel Amoah, Dr. R. Long, Dr. J. Yan, M. V. M. Prashant

The formation of functionalized self-assembled monolayers (SAMs) on surfaces for biosensors, medical diagnostics, and nanostructured materials is currently the subject of intense investigation. In our effort to develop an electrochemical biosensor with high sensitivity and portability, we propose a transducer molecule with viologen in the middle for redox sensing, a sulfhydryl group at one end for adsorption on a gold electrode surface, and a biotin group at the other end for sensing of avidin.

We have completed the first two of six steps in the synthetic route, and the products have been purified and characterized. First, thioacetic acid was added to 11-bromoundecene under photochemical conditions. The product was then reacted with 4,4 -bipyridine (nucleophilic displacement of bromine) to obtain a monoquaternarized product. We then perform methanolysis to convert the thioester group to a

mercapto group.

Subsequent self-assembly of this product with 1-mercaptoundec-11-yl tri(ethyleneglycol) on gold electrode surface will form a mixed SAM. Surface diquaternerization of the exposed pyridine group with 2-aminoethylenebromide will form the viologen group (i.e., 4,4 -bipyridyl). biotin will then be attached to the amino group at the monolayer through amide bond formation. This approach will produce this complex transducer molecule in higher purity and yield than would be possible with solution phase synthesis. The modified electrode will be used for reagentless biorecognition of avidin in solution. Transduction of the biorecognition is achieved by the changes in the redox properties of the viologen groups resulting from the binding.

Jithendra R. Bonthu
Graduate Student
Chemistry

"Tethering Single Lipid Bilayers inside Nanopores of Anodic Aluminum Oxide for Multinuclear NMR Studies."
Authors: Jithendra R. Bonth and Juchao Yan

The aim of this research is to develop a reliable method of forming nanopore-confined single lipid bilayers (SLBs) for solid-state nuclear magnetic resonance (NMR) spectroscopic studies. Specifically, the small unilamellar vesicles, consisting of one biotinylated lipid and another chain-deuterated lipid, will be attached to cylindrical nanopores of anodic aluminum oxide (AAO) through the high affinity of streptavidin towards the biotinylated lipid. Then, vesicle fusion forms confined SLBs in a fluid state. 1H-magic angle spinning (MAS) NMR will be used to extract the structural information and 2H- and 31P-MAS NMR will be used to extract orientational information of the resulting SLBs. This work is driven by two current needs. One is to build robust biochip and biosensor assays. The other is to develop patterned deposition of lipids and membrane-associated proteins.

Commercially available AAO membranes (i.e., Anodiscs®) have only three nominal pore diameters (0.02, 0.1, 0.2 μm). The nanopores of Anodiscs® are not perfect cylinders, and are not perfectly coaxial. In our laboratory, we are fabricating freestanding AAO membranes with oriented through-holes. The pore features, including diameters, depths, and porosities, will be specifically manipulated to achieve a spectrum of nanopore arrays. After fabricating sufficient freestanding AAO membranes, we will tether SLBs inside the nanopores through vesicle docking and subsequent vesicle fusion. Then, we will stack about one hundred fully hydrated AAO membranes with tethered SLBs into a MAS rotor and fill it with either deuterium-depleted water or buffer for solid-state NMR studies.

New Mexico Highlands University

Victor Khrustalev
Graduate Student
Chemistry

"New mixed main group-transition metal chalcogenides"
Authors: Sergey V. Savilov, Mikhail Yu. Antipin, and Tatiana V. Timofeeva

Infinite systems of bonds between metal atoms remain intriguing objects for many researchers demonstrating a rich and surprising structural chemistry and interesting physical properties. Striking illustrations are the mixed metal-rich chalcogenides of early transition metals, which form a wide variety of heterometallic frameworks ranging from 1D chains in M4ETe4 (M = Nb, Ta; E = Si, Cr, Fe, Co, Ni) to 3D frameworks in Ta9M2S6 (M = Fe, Co, Ni). Mixed transition-rare earth, metal-rich chalcogenides also have a developed structural chemistry {1D chains in Sc14M3Te8 (M = Ru, Os), 2D slabs in Sc6MTe2 (M = Cu, Ag, Cd), 3D frameworks in Er7Ni2Te23}. At the same time, mixed metal-rich chalcogenides of main group and transition metals are much less studied. For the systematic investigation of main group-transition metal mixed chalcogenides, new phases in the Ni-Sn-Q and Pd-Sb-Q (Q = chalcogen) systems have been synthesized and its crystal structure determined by X-ray crystallography. This work also reports their physical (conductivity and magnetic susceptibility) properties as well as electronic structure and bonding.

Tiffany Kinnibrugh, Tiffany L Kinnibrugh, Andrey A Yakovenko, Victor N Khrustalev, Mikhail Yu Antipin, Tatyana V Timofeeva
Various
Chemistry

"Nano-porous-Metal-Organic Frameworks "
Authors: Tiffany Kinnibrugh, Tiffany L Kinnibrugh, Andrey A Yakovenko, Victor N Khrustalev, Mikhail Yu Antipin and Tatyana V Timofeeva

X-ray structural investigations of Metal-Organic Frameworks (MOF) synthesized at Sandia NL and Los Alamos NL are presented. For several MOFs fluorescent trans-stilbene ligand was used. For one MOF interpenetrated lattice very large cavity was found.

New Mexico State University

Sami A. Al-Haddad
Graduate Student
New Mexico State University

"Estimating Seepage from Irrigation Canals Before and After Pipeline Installation in the Elephant Butte Irrigation District, New Mexico"
Authors: Sami A. Al-Haddad, Henry Magallanez, J. Phillip King, and A. Salim Bawazir

In response to persistent drought conditions in New Mexico, Elephant Butte Irrigation District (EBID) initiated its water conservation project in 2003 by installing pipelines in earthen irrigation laterals in an effort to control seepage losses. This study was conducted to estimate seepage losses from the targeted laterals before and after the installation of pipelines. Two methods were used in this study to estimate seepage losses; an experimental approach using the ponding method and theoretical approach using the Vedernikov's method.

The results from this study, using the ponding method, indicated that the measured unit water losses from the laterals ranged from 0.96 to 4.55 ft^3/ft^2/day and from the pipelines ranged from 0.15 to 0.38 ft^3/ft^2/day. The efficiency of the pipelines, in terms of water salvage, ranged from 60% to 97% with an average of 86%. The estimated seepage using Vedernikov's method ranged from 1.74 to 3.32 ft^3/ft^2/day with an average of 2.40 ft^3/ft^2/day.

The study concluded that there is a great potential for water conservation and improvement of off-farm conveyance efficiency by installing pipelines. It demonstrated that seepage losses could be reasonably estimated using Vedernikov's method.

Sourav Adak and Boris Kiefer
Graduate Student and Assistant Professor
Civil Engineering

"The Equation of State of α-Uranium from a First Principles Perspective"
Authors: Sourav Adak and Dr. Boris Kiefer

Uranium occurs in diverse environments, for example as a fuel in nuclear reactors and as a major source for the internal heating of our planet. Therefore the understanding of the electronic structure of uranium is important to develop a unified model for uranium in different bonding environments. Heavy elements at the bottom of the periodic table pose a large challenge to theory due to the often complex interplay of s-, d-, and f-electrons that are difficult to treat self-consistently in density functional theory. Here we adopt the simplest description that neglects spin-orbit coupling and any special treatment of strong electronic correlations. The calculations are based on the projected augmented wave method within the GGA approximation. We find that the equation of state is in good agreement with experiment. This suggests that our simplified electronic structure model of uranium captures most of the physics and may be used to describe
bonding of this element in other environments at least to first order.

Kate Adams and Zack Libbin
Graduate Student and Undergraduate Student
Civil Engineering

"Evapotranspiration Estimates Based on Standardized Equation Referenced to Grass using New Mexico Weather Station Data"
Authors: Kate Adams and Zack Libbin

Several methods such as the Blaney-Criddle, Modified Penman, pan evaporation and others are commonly used to determine evapotranspiration (ETref) of a reference crop such as alfalfa or grass. Many of these methods used are empirical methods and are calibrated for certain regions with specific climates; therefore their use is limited to localized conditions. In order to apply these methods to other regions with different climates, extensive research is necessary to re-calibrate these methods.

Computation of reference ET using a standardized method has been proposed by the Committee of the Environmental and Water Resources Institute of American Society of Civil Engineers (Allen et al., 2005). The proposed method sets a benchmark equation that standardizes the calculation of ETref and improves transferability of crop (Kc=ETactual/ETref) coefficients. The standardized equation requires meteorological data from local weather stations, such as wind speed, relative humidity, air temperature and solar radiation. However, this method also requires stringent conditions at the location of weather stations. These conditions assume a dense reference crop, well-watered, free of disease, of a specific height and fetch distance. Many weather stations in New Mexico do not meet these requirements. Reference ET by standardized equation using meteorological data from weather stations located in New Mexico was investigated.

Stefanie L. Japel and Boris Kiefer
Postdoctoral Researcher
Physics

"FeP at pressures up to 70GPa, phase transitions, magnetic structure, and EOS."
Authors: Stefanie L. Japel and Dr. Boris Kiefer

Iron Phosphide FeP occurs in several different planetary environments. Geochemical and cosmochemical models suggest the presence of FeP in the Earth's Core at pressures between 137 and 371 GPa. At much lower pressure (about 25GPa) FeP is of interest because of the comparatively high levels of P in its Fe-rich mantle, FeP may contain clues as to the petrological evolution of Mars.

X-ray diffraction experiments on the iron phosphide FeP indicate that a phase transition occurs in the material from the metallic MnP structure to the FeS(III) structure. Because of the breadth of the diffraction peaks, and due to a very large (approximately 10GPa) range of coexistence of the two phases, it has been difficult to determine at which pressure the phase transition actually occurs.

In order to understand the electronic and magnetic properties with compression, we have performed first-principles calculations, comparing FeP and FeS which have several similar crystal structures. Our preliminary result for the MnP (room temperature and pressure) phase of FeP show that this material is an antiferromagnet, as is the corresponding (FeS-II) phase. The combination of experiment and theory shows that magnetism in the FeP system may be present up to at least 25 GPa, a factor of 2 higher as compared to the FeS system.

Brad Kirksey
Undergraduate Student
Civil Engineering

"Crop Evapotranspiration Study for Dona Ana County, New Mexico"
Authors: Brad Kirksey, A. Salim Bawazir, Zohrab A. Samani, and Max Bleiweiss

Water in the Southwest is scarce and the demand for fresh water for supplying the urban population, irrigation, and habitat requirements is on the rise. In Doña Ana County, New Mexico, irrigation is the largest consumer of water, yet the consumptive use by crops has not been reliably quantified. In the ongoing stream adjudication, the New Mexico Office of the State Engineer (OSE) currently uses a simple Soil Conservation Service (SCS) Modified Blaney-Criddle equation (Blaney and Hanson 1965) to estimate agricultural consumptive use by crops in the County.

As the population of the County grows, it is becoming increasingly necessary to plan and prepare for converting domestic, municipal and industrial water supplies from complete dependence on groundwater to conjunctive use of surface water and groundwater. Therefore, a better estimate of agricultural consumptive use is necessary. Consumptive use or evapotranspiration (ET) is considered a loss from hydrologic water balance. This study measured evapotranspiration (ET) of pecans by eddy covariance technique in 2006 and, in addition, quantified the consumptive use of water by crops in the County using 2002 remote sensing data.

Eric Lopez
Graduate Student
Civil Engineering

"Wind Profile in a Pecan Orchard, Dona Ana County, New Mexico"
Authors: Dr. Salim Bawazir, Dr. Zohrab Samani, and Eric Lopez

The structural roughness of pecan trees, open space between the rows, and the fetch distance from the edge of the field are known to affect the vertical wind profile within the canopy and thus affect evapotranspiration rates. This study investigated the vertical profile of horizontal wind velocity in a pecan orchard in Dona Ana County, New Mexico.

A vertical wind profile investigation was conducted using multiple anemometers (wind speed sensors). The purpose of this study was to determine if the vertical wind profile in a pecan orchard was logarithmic, like the wind profile in short crops. Data was collected and analyzed using a graphical method. The results confirmed the hypothesis that the wind profile in the orchard was logarithmic. Friction velocity and shearing stress were also calculated from the same data. However, since only one type of sensor, with quite a variation in accuracy, was used further studies are required. Using a newer, technologically advanced, three dimensional sonic anemometer,

wind measurements can be made in three dimensions and at high frequencies. These measurements will allow for the calculation of friction velocity and shearing stress. Results from the three dimensional sensor will be used to validate the graphical method.

Ernesto Santillano
Undergraduate Student
Civil Engineering

"Soil Chemistry of Areas Occupied by Saltcedar at the Elephant Butte Delta"
Author: Ernesto Santillano

Soil chemistry of areas occupied by saltcedar at the Elephant Butte Delta was studied. The study site included non-treated and herbicide-treated saltcedar. At the treated site, saltcedar was dead but still standing. At each site four areas were selected randomly to collect soil samples for laboratory analysis and also to measure conductivity, dissolved solids, and temperature. Preliminary results from both field measurements and the laboratory analysis indicated that there is more salt in the untreated saltcedar site than the treated saltcedar site. The soils in this were slightly alkaline (pH of 7.3 to 7.4). The salinity (EC) levels in the untreated site decreased as the leaves senesced but then increased as the leaves decomposed. Recent measurements show that after bud break in the non-treated site, the EC continues to increase. There was no indication of sodium related problems as both sites (SAR < 13).

Jose A. Solis
Graduate Student
New Mexico State University

"Evapotranspiration of Treated and Non-Treated Saltcedar"
Author: Jose A. Solis

This study focuses on a major concern by the United States Bureau of Reclamation (USBOR) and the Interstate Stream Commission as to whether sufficient amounts of water lost due to evapotranspiration (ET) can be reduced by the clearing of saltcedar (*Tamarix ramosissima*) in riparian dominated areas. Saltcedar is known to consume large amounts of water (1.3 hectare-m per hectare per year) and its control is very expensive. The USBOR has undertaken an effort to control it by treating a large area with herbicide. Part of the area was left untreated in order to estimate the water use by saltcedar in both a treated and untreated area. At both sites, two systems were used to measure the ET of the saltcedar. One of the systems is the OPEC (one propeller eddy covariance) system, and the other system is the 3D-SEC (3-dimensional sonic eddy covariance) system. Measurements of ET from both sites indicated that the treated saltcedar stand during a comparison of 83 growing days was less than the non-treated site by about 57%.The ET measured at the treated site was not equal to zero due to soil evaporation.

University of New Mexico

Alandren Etlantus
Graduate Student
Civil Engineering

"Estimating Evapotranspiration With Remote Sensing Scaling: How It Works, How It Compares"
Author: Alandren Etlantus

This poster will present background on scaling evapotranspiration (ET) in the riparian corridor of the middle Rio Grande as well the status of comparison between the Scaling method and the methods used by other NMEPCoR researchers to remotely sense ET in the middle Rio Grande. ET estimates from the scaling method for the Riparian Corridor of Bosque del Apache National Wildlife Refuge, NM on May 31, 2002 has been compared to estimates from the Surface Energy Balance Algorithm For Land (SEBALNM), Regional ET Estimation Model (REEM) and ET estimation with MODIS methods. The initial comparison results show some variability among the methods and demonstrated the need for the comparison of additional dates and locations. Dates and locations have been selected for the additional comparison. In addition, the first comparison indicated the need for consistent preparation and georectification of the imagery. The scaling team is currently performing radiometric corrections and georectification of Landsat 7 images for the dates selected. These images will be shared with all researchers for use with the other models where possible. Once ET estimates for the new dates and locations have been completed for each method, comparison of the estimates will be made.

Alicia Paz-Solis
Graduate Student
Civil Engineering

"Interpretation of Ground and Satellite Based Data to Estimate Evapotranspiration (ET) along the Middle Rio Grande"
Author: Alicia Paz-Solis

This poster is an interpretation in English and Spanish of the connection between ground and satellite based measurement of ET along the Middle Rio Grande (MRG).

The study of ET is important in semiarid regions like New Mexico because much of the water available for consumption is depleted through the evapotranspiration process. In fact, estimates of ET along the MRG reach range from 20 to 50% of the total water budget. As water managers attempt to minimize water losses, the challenge for scientists extends beyond simply quantifying ET. Scientists need to attribute ET depletions to complex landscape structure and function in order to determine how best to restrict these depletions. Ground based climatic data are collected using four instrumentation towers installed in representative ecosystems. The data form the basis for calculating ET using the eddy covariance method. ET is then scaled from a leaf area perspective.

Specifically, it relates ET to a measure of leaf area index (LAI) and constructs a model that accounts for canopy subclasses, climate, and landscape topography. Field measurements of LAI are based on a remotely sensed vegetation index (VI) derived from Landsat 7 Enhanced Thematic Mapper Plus imagery. Leaf Area Index (LAI) is a key biophysical variable influencing land surface photosynthesis and transpiration and can be related to remotely sensed data.

Jamie Reed and Danielle Garcia
Graduate Student
Chemical Engineering

"Thermally Responsive Cell Culture Substrata for Systems Biology and Drug Discovery"
Author: Jamie Reed

Epidermal growth factor receptor (EGFR) is key receptor embedded in the plasma membrane of cells. EGFR is often up-regulated in cancer cells, resulting in uncontrollable cell growth and metastasis. Cells expressing high levels of EGFR are therefore often used as an in vitro model system for monitoring the efficacy of new cancer therapeutics using techniques such as flow cytometry (FC). However, cells expressing EGFR are highly adherent to both the substrate and each other. The methods traditionally used to detach cells from surfaces destroy the integrity of proteins in the extracellular matrix (ECM), resulting in damaged protein and receptors, making them incompatible with the solution-based analysis. In this work, we describe the use a thermo-responsive polymer, poly(N-isopropyl acrylamide) (pNIPAM), for non-destructive release of cells into suspension, where they may ultimately be analyzed by techniques such as FC. To optimize the pNIPAM substrates, pNIPAM films were prepared using different methods (e.g., plasma vs. solution deposisiton) and compositions (10 and 20 wt% pNIPAM). The surface chemistry of the resulting films were characterized using X-ray photoelectron spectroscopy (XPS) and the thermoresponsivity was determined by contact angle analysis. In addition, the behavior of a variety of cells were tested, including baby hamster kidney (BHK) and patient-derived endothelial cancer cells expressing increased levels of EGFR (A431). We found the best detachment behavior for BHK cells from 20wt% pNIPAM/silica surfaces. However, it is predicted that the best cell release will be from plasma deposited pNIPAM surfaces, where we also find that the surface chemistry is that which most closely resembles that of the theoretical composition of the monomer. Future applications of this technology could be used to release single cells for measurement of cell surface markers by FC and cell sheets to measure cell-cell adhesion.