ND EPSCoR 2021 State Conference

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Acknowledgments

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New Discoveries in the Advanced Interface of Computation, Engineering, and Science (ND-ACES)

Early Cancer Detection by Cell-Free Chromatin and AI

Motoki Takaku, Xusheng Wang, Alyssa Erickson, University of North Dakota Department of Biomedical Sciences

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

Cell-free DNA (cfDNA) has become a very promising biomarker for early detection of tumors. CfDNAs are known to partially retain epigenetic information such as DNA methylation and chromatin structures. Such epigenetic information can be used to predict cell-of-origin and thereby cancerous tissues. In this pilot project, we plan to collect cfDNA data from human cancer patients and identify specific features in cfDNAs. Using our own and published data, we will establish a machine-learning based tool.

High-Fidelity Simulation of Flows in Bone-Like Environment to Investigate the Growth of Cancer Cells

Lahcen Akerkouch, Haneesh Jasuja, Luke Kieffer, Davina Kasperski, Ethan Wells, Dinesh Katti, Kalpana Katti, Trung Bao Le, North Dakota State University Civil and Environmental Engineering Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

We investigate the role of interstitial fluid flow on the growth of cancer cells within the interconnected pores of human bone. In-vitro experiments were carried out in a bio-reactor that includes bone-like scaffolds. We created a full-scale 3D model of the scaffold based on the micro-CT data. We performed Computational Fluid Dynamics simulations to investigate the flow patterns inside the pores of the scaffolds. The results reveal non-uniform distributions of flow velocity and shear stresses.

Simulating Functional Behavior of Graphene-Based Biosensors Detecting Toxic Hydrogen Sulfide Gases

Rebecca Tomann and Svetlana Kilina, North Dakota State University Chemistry and Biochemistry Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

We have modeled nanopatterned holey graphene (HG) substrate electronically hybridized with Au nanoparticles, using density functional theory. Adsorption of H2S on the HG-Au distorts H2S molecules. Such conformational changes significantly affect the electronic states near the energy Fermi, which are reflected in DC-conductivity. The results prove the ability of HG/Au-nanoparticle systems working as an electronic sensor for detecting toxic H2S gas even at its small concentrations, when only a few H2S molecules are present.

Coarse-Grained Modeling of Mechanical Behavior of Montmorillonite Clay

Sarah Ghazanfari, H. M. Nasrullah Faisal, Kalpana S. Katti, Dinesh R. Katti, Wenjie Xia, North Dakota State University Civil and Environmental Engineering Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

Sodium montmorillonite (Na-MMT) clay is one of the constituents of expansive soils which plays

an important role in swelling. In this study, we employed Molecular Dynamics (MD) to analyze the physical behavior of (Na-MMT). To this end, we implemented a coarse-grained molecular dynamics simulation, which provides an efficient approach to study materials at a fundamental molecular level. Furthermore, we utilized Steered Molecular Dynamic (SMD) to investigate the mechanical properties of a coarse-grained model of montmorillonite.

Machine Learning Algorithms for the Identification of Cancerous Tumors

Solene Bechelli, Jerome Delhommelle, University of North Dakota Chemistry Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

In this study, we investigate the relevance of Machine Learning Algorithms (MLA) for the detection of cancerous tumors through image detection. We compare the performance of linear models (Logistic regression, Linear Discriminant Analysis), classification models (K Neighbors Classifier, Decision Tree Classifier) and Naive Bayes (Gaussian NB). In addition, we look at the performance of Convolutional Neural Networks (CNN). Our results point toward a better accuracy of the CNN model.

Promoting Retention and STEM Success Through Research Training Groups

Andrea Doyon, Georgia Paul, Sarah Sletten, University of North Dakota Counseling Psychology Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

The current study aims to evaluate the effectiveness of a vertically integrated support system-Research Training Groups-directed at helping retain college students and promoting their success at future STEM researchers. During this multi-year study, participants will complete baseline and follow-up surveys pertaining to their professional/technical skills, self-efficacy, persistence intentions, sense of belonging, and formative assessment. Participants are also invited to mentorship activities and will be rewarded via a digital badging process.

A Hybrid Continuum-Particle Approach for Fluid-Structure Interaction Simulation of Red Blood Cells in Fluid Flows

Lahcen Akerkouch, Trung Bao Le, North Dakota State University Civil Engineering Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

The motion of cells through microchannels has been an active research topic over the last decade. However, results revealed that experimental methods alone are not capable to accurately model the cellular dynamics. In this work, we developed new a hybrid-continuum approach coupled between the immersed boundary method and the Dissipative Particle Dynamics. Our results showed the rigorousness of the new model, following the deformation of the cell with fulfilling the incompressibility condition of the flow.

A Runtime Performance Analysis of a Traditional and Virtual HPC at UND

Zakaria El Mrabet, David Apostal, Aaron Bergstrom, University of North Dakota Electrical Engineering and Computer Science Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

High Performance Computing (HPC) systems have been useful to scientists by decreasing

program runtimes. Virtual HPC systems allow users to create customized computing environments that would be difficult to create in traditional HPC systems. In this study, we compare the runtime performance of a virtual HPC system to that of a traditional HPC system.

Metarrestin-Encapsulated Polymeric Nanoparticles for Drug Delivery to Breast Cancer Bone Metastasis

Babak Mamnoon, Sanku Mallik, North Dakota State University Pharmaceutical Sciences Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

Triple-negative breast cancer is one of the most aggressive types of cancer due to its recurrence including and metastasis to different organs bone. Low oxygen content (hypoxia) in tumors contributes to overall resistance to chemotherapy and radiation therapy. In this study, we prepared metarrestin-encapsulated polymeric nanoparticles (polymersomes) to deliver anti-metastatic drug into hypoxic solid tumors.

The Mechanics of Integrin Molecules and their Role in Cell Differentiation

Hanmant Gaikwad, Sharad Jaswandkar, H. M. Nasrullah Faisal, Kalpana Katti, Dinesh Katti, North Dakota State University Materials and Nanotechnology Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

The Integrins couple the extracellular matrix to the cell cytoskeleton and facilitates cell migration, proliferation, and differentiation. Their role as mechanotransducer and signaling molecules implicates the cancer progression from the primary tumor to metastasis. For investigating the mechanotransduction of integrin in cell adhesion, simulation of integrin has been carried out using steered molecular dynamics. Also, the interaction between integrin and Na-montmorillonite clay has been studied to evaluate the osteoconductivity and cell differentiation mechanism.

Computational Studies on Nonnatural Amino Acids

Atir Kaunain, Hui Pu, Tao Yu, University of North Dakota Petroleum Engineering Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

In this study, we employed the density functional theory method to investigate structures and properties of six non-natural amino acids (NAA). Using Gaussian09, we optimized the geometries of NAA in the gas and aqueous solution phases. The atomic charges of NAA were calculated, and this information will be useful to understanding the nonbinding interactions between NAA and clay materials. Meanwhile, the HOMO and LUMO orbital information of each NAA is also investigated.

Map of Topics and Concepts Addressed in ND-ACES Bioscience Module 1: Cellular Scaffolding

Sameera Algarni, Ryan Summers, Addison Beaty, Mckenzie Belfiori, University of North Dakota Teaching, Leadership, and Professional Practice Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

During ND-ACES Year 1, Education and Workforce Development faculty and research assistants have planned and assembled a bioscience module. This module is designed to

support teaching and learning about cellular biology topics resembling the research activities in the CCSBE Cellular Pillar. This module centers on cellular scaffolding, connecting to cell structure and function content goals for pre-college biology instruction. Specific concepts include: Cell and tissue organization; immune responses; tissue engineering; and biological polymers.

Nanoclay based Bone-Mimetic Scaffolds in Perfusion bioreactor Enabled 3D In Vitro Model of Prostate Cancer Bone Metastasis

Haneesh Jasuja, Dinesh R. Katti, Kalpana S. Katti, North Dakota State University Civil and Environmental Engineering Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202, NDSU Grand Challenge Center for Engineered Cancer Test Beds

Three-dimensional (3D) dynamic tumor models help elucidate cancer mechanisms as they accurately recreate complex multicellular organization and the dynamic interactions of microenvironment instead of a static culture that suffers from lack of role of shear forces and uneven nutrient supply. In this study, we developed 3D-dynamic in vitro model of prostate cancer bone metastasis using nanoclay-based scaffolds and a perfusion bioreactor. We performed various cellular assays and immunocytochemistry to establish the feasibility of dynamic culture.

Polymeric Scaffold with Wheat Bran Arabinoxylan for Tissue Engineering

Hayle Boechler, Taylor Stegman, Brooke Roeges, Khwaja Hossain, Mayville State University Biology Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

Wheat bran biopolymer can be used in the preparation of scaffold for tissue engineering. Arabinoxylan was extracted from wheat bran. Various concentrations of arabinoxylan will be mixed with chitosan and polygalacturonic acid separately. The prepared scaffolds will be analyzed for mechanical strength, porosity, and surface chemistry. Resulting scaffolds with adequate mechanical properties may determine the suitability of using arabinoxylan in bioactive polymeric scaffolds that can mimic native environment for human cell culture and engineering.

The Effects of Arabinoxylan on Gut Flora Immunity

Taylor Stegman, Brooke Roeges, Hayle Boechler, Khwaja Hossain, Michael Kjelland, Sean Pollack, Mayville State University Biology Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

Bacteria in the gut, while attributing to digestion, also has an effect on immunity. Arabinoxylan (AX) has been reported to contain immunomodulatory activity, as well as other health benefits. Wheat bran is an excellent source of AX and was used to extract this fiber. Different concentrations of AX and its derivatives will be used in the media for culturing bacteria to study the effects of AX on the growth and development of beneficial gut bacteria.

Uncovering the Dynamical Features of Actin Filament Contributing to its Strength and ADF/Cofilin Mediated Severing Process: A Steered Molecular Dynamics Approach

Sharad V. Jaswandkar, Kalpana S. Katti, Dinesh R. Katti, North Dakota State University Materials and Nanotechnology Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202, NDSU Grand Challenge funded Center for Engineered Cancer Testbeds, NSF

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Actin is involved in various eukaryotic cells' functions due to its abundance and intrinsic ability to transition between a monomeric and polymeric form. Understanding how actin contributes to highly organized and complex processes continues to be a significant focus of research across multiple disciplines. In the present study, steered molecular dynamics (SMD) simulations approach is utilized to explore actin filament mechanics and its ADF/Cofilin mediated severing mechanism.

Breast Cancer Image Segmentation with U-net

Chanaka Sampath Cooray Bulathsinghalage, Lu Liu, North Dakota State University Computer Science Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

Applying machine learning techniques in medical images promises potentially better disease diagnosis. In this study, U-net segmentation network is used to segment the regions of interest from the breast cancer mammogram images. U-net is based on fully convolutional neural network used for image segmentation and optimized to work with fewer training images. The datasets used to train and test this model are MIAS and DDSM, two popular breast cancer mammogram image data sets.

Rhodiola Crenulata Induces Cytotoxicity in Bone Metastatic Breast Cancer Grown on 3D In Vitro Nano-clay Based Bone Mimetic Scaffold

Preetham Ravi, Haneesh Jasuja, Dipayan Sarkar, Kalidas Shetty, Dinesh R. Katti, Kalpana S. Katti, North Dakota State University Materials and Nanotechnology/Civil Engineering Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202, NDSU Grand Challenge Center for Engineered Cancer Test Beds

Rhodiola crenulata is a tibetan plant-based extract that is recently shown to be effective for primary site breast cancer. Bone metastatic breast cancer is a fatal disease in which many of the available anticancer therapeutics are ineffective due to lack of appropriate models. In this study, we tested Rhodiola crenulata on our 3D in vitro model of breast cancer bone metastasis. We have performed various cellular bioassays to observe the cytotoxicity of Rhodiola crenulate.

Efficacy of Metarrestin for Bone Metastatic Breast Cancer Evaluated Using 3D In Vitro Bone Mimetic Testbed

Sibanwita Mohanty, Preetham Ravi, Haneesh Jasuja, Dinesh R. Katti, Kalpana S. Katti, North Dakota State University Materials and Nanotechnology/Civil Engineering Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202, NDSU Grand Challenge Center for Engineered Cancer Test Beds

Bone metastatic breast cancer is the leading cause of breast cancer deaths due to poor prognosis. Metarrestin is a perinucleolar compartment inhibitor which has been tested on primary site pancreatic, prostate, and breast cancer. However its efficacy for bone metastatic breast cancer is still undefined. In this study, we developed a 3D in vitro bone metastatic breast cancer model using nanoclay based scaffolds to elucidate the cytotoxic effects of Metarrestin on bone metastasized breast cancer.

Breast Cancer Image Classification with Deep Learning

Megan Heeren, Lu Liu, North Dakota State University Computer Science Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-

1946202

Mammography is the most used method to detect breast cancer, which affects women worldwide. The increasing number of mammogram images places a great burden on radiologists. As the advancement in technology, machine learning gives the promise of classifying medical images automatically. In this project, we apply deep learning algorithms on a popular breast cancer image data set and compare their performance with other machine learning algorithms.

Establishing and Characterizing Patient-Derived Breast Cancer Cell Lines

Farid Solaymani Mohammadi, North Dakota State University Biological Sciences Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202, NDSU Grand Challenge Center for Engineered Cancer Test Beds

Patient-derived cancer cell lines are irreplaceable resources to reflect human cancer's nature and to develop personalized medicines. To validate the capacity of 3D in vitro testbed of breast cancer for Patient-derived cancer cells, we have isolated and characterized breast cancer cells from 6 patients. We optimized culture conditions, passaging methods, and cancer cell purification techniques. Each cell line was verified for the presence of cytokeratin-19 (CK-19), which is highly expressed in breast cancer cells.

Synergistic Effects of All-trans Retinoic Acid (ATRA) on Triple Negative Breast Cancer Cells

Madison Koppelman, Jacob Shreffler, Sanku Mallik, North Dakota State University Pharmacy/Pharmaceutical Science Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

Triple-negative breast cancer (TNBC) is the deadliest breast malignancy and comprises 10-15% of cases. Solid tumors develop early and harbor drug-resistant cancer stem cells (CSC). All-trans Retinoic Acid (ATRA) induces differentiation of CSC in a variety of solid tumors. Herein, we demonstrate the synergistic effect of Doxorubicin and ATRA on cytotoxicity of TNBC cells in a monolayer and describe the methods of ATRA quantifications by High-performance Liquid Chromatography (HPLC).

Leveraging Transfer Learning on Classifying Breast Cancer Images

Clayton Klemm, Lu Liu, North Dakota State University Computer Science Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

The best way to treat breast cancer is by early detection. The aim of this project is to use Machine Learning (ML) to computationally learn how to detect and classify breast cancer mammogram images. Specifically focusing on whether or not cancer exists and if it exists what is its type (benign, malignant). The overall goal is to use a pretrained model, such as resnet50, and use different transfer learning techniques to train it.

Breast Cancer Image Analysis with Autoencoder

Ansley Schug, Lu Liu, North Dakota State University Computer Science Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

Breast cancer affects women worldwide. Early detection of malignant abnormalities is imperative in treating it. Machine learning can be used as a tool for detecting benign or

malignant breast tumors. This project uses an artificial neural network called an autoencoder to encode and decode breast cancer images. With this unsupervised learning approach, the autoencoder will learn patterns in the images and use this information to detect benign or malignant breast abnormalities.

A Novel Sensitivity Analysis-Based Method for Feature Selection using Feed-Forward Neural Networks

Dayakar Naik Lavadiya, Ravi Kiran Yellavajjala, North Dakota State University Civil Engineering Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

Feature Selection is a pre-processing step often carried out to enhance the performance of machine learning algorithms. This study proposes a novel sensitivity analysis-based approach which employs a complex-step derivative approximation scheme in the framework of feed-forward neural networks for feature selection. Real-world datasets for classification and regression tasks are chosen, and the efficacy of proposed method is demonstrated. Furthermore, other feature selection methods are employed, and results obtained from the proposed method are compared.

Investigation of the Mechanical Behavior of Swelling Clay Tactoid

H. M. Nasrullah Faisal, Kalpana S. Katti, Dinesh R. Katti, North Dakota State University Materials and Nanotechnology Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202, CCAST

Swelling clays have been focus of researchers because of their impact and application in variety of fields such as geotechnical, environmental, structural nanocomposites and tissue engineering. Tactoid, formed by vertical stacking of several clay mineral layers, is considered as the most important level of clay hierarchical structure. Investigation of dry and hydrated tactoid using molecular dynamics simulations are conducted to understand the impact of hydration on mechanical behavior of tactoid and expounding the underlying mechanisms.

Comparison of SARS-CoV and SARS-CoV-2 (COVID-19) Viral Replication Complexes

H. M. Nasrullah Faisal, Kalpana S. Katti, Dinesh R. Katti, North Dakota State University Materials and Nanotechnology Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202, CCAST

SARS-CoV-2, the contributing virus of the current global pandemic COVID-19, shows an analogous viral life cycle with the previously originated coronavirus SARS-CoV, but with dramatically different outcomes. Both coronaviruses employ viral replication complex to carry out their viral replication and transcription. As protein-protein non-bonded interactions contribute to the different biological processes, investigation of non-structural protein interactions within the coronaviral replication complex by molecular dynamics simulations can potentially allude to their differences in replication behavior.

3D In Vitro Nanoclay-Based Breast Cancer Bone Metastasis Testbed Using Patient-Derived Tissues

Haneesh Jasuja, Farid Solaymani Mohammadi, Jiha Kim, Anu Gaba, Dinesh R. Katti, Kalpana S. Katti, North Dakota State University Materials and Nanotechnology Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-

1946202, NDSU Grand Challenge Center for Engineered Cancer Test Beds, NIH U54GM128729

3D in vitro models have the potential to recapitulate human tumor biology to gain better insight into tumor progression, provide personalized therapies and screen new drugs. We have successfully developed a 3D in vitro testbed of breast cancer bone metastasis using nanoclay based scaffolds. Here we demonstrate the validation of the testbed model by employing patient-derived breast cancer cells. Results on characteristics of testbed derived tumors using patient derived cells are presented.

Polymer Nanocomposite Fiber-Based Scaffolds for Bone Tissue Engineering

Krishna Kundu, Ayda Afshar, Dinesh R. Katti, Mohan Edirisinghe, Kalpana S. Katti, North Dakota State University Civil and Environmental Engineering Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202, ND Department of Commerce (Grant 19-11-G-237, NSF, UK Engineering and Physical Sciences Research Council (Grants: EP/S016872/1, EP/N034228/1, and EP/L023059/1)).

The present study focuses on the development of nanoclay based polymer composite nanofibers using a novel fabrication method called pressurized gyration (PG) for bone tissue engineering applications. We observed enhanced cell viability, osteogenic differentiation, ECM formation, and collagen formation for the PCL HAP MMT-Clay nanocomposite fiber scaffolds compared to the pristine PCL fibers. These studies represent a new opportunity in the design of manufacturable composite nanoclay polymer fibers for bone tissue engineering applications.

Characterizing the Mechanical Properties of ASTM A36 Steel Metallurgical Phases Using Clustering Analysis

Dharanidharan Arumugam, Dayakar L. Naik, Ravi Kiran, North Dakota State University Civil and Environmental Engineering Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

The study aims to evaluate the nanomechanical properties of ferrite and pearlite phases present in the ASTM A36 steel. We performed K++ means clustering on 1575 observations with two descriptive features, namely hardness and Young's modulus obtained through the nanoindentation of seven different heat-treated A36 specimens. The determined mean hardness and Young's modulus of ferrite were 2.68GPa and 205.3GPa, and for pearlite, 3.64GPa and 204.0GPa, respectively.

Synthesis and Characterization of Nanocomposite for Cancer Cell Culture

Lexi Carpenter, Sean Pollack, Raj Hazra, Mohiuddin Quadir, Khwaja Hossain, Mayville State University Biology Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

The structural stability and environment of bioactive scaffold mimic the functionality of native tissue and could be used for cellular regeneration. Chitosan (Chi) and Polygalacturonic Acid (PgA) were dissolved in diluted acetic acid and sodium hydroxide and separate solutions were prepared in deionized water. Several scaffolds were prepared by mixing Chi and PgA solutions followed by sonication. The mechanical properties showed that the prepared ChiPgA scaffolds could potentially be used in cancer cell regeneration.

Center for Regional Climate Studies (CRCS)

The Oakville Prairie Mesonet

Aaron Kennedy, Alec Sczepanski, and James Hyde, University of North Dakota Department of Atmospheric Sciences

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

The recently installed Oakville Prairie Mesonet is described. Metoeorlogical instrumentation supports multidisciplinary research at the Oakville Prairie Field Station / Observatory, local stakeholders, and hazardous weather research. The site also serves as a testbed for experimental instrumentation. The author has partnered with OTT Hydromet who is using the facility as a winter testing ground for some of their instrumentation.

Air Quality Study at Nueta Hidatsa Sahnish College, Fort Berthold Reservation, North Dakota

Janna Steen, Tyler Hanson, Lizette Alvarez, James Medeiros, Montserrat Rodriguez, Kerry Hartmann, and Bernhardt Saini-Eidukat, North Dakota State University Geosciences Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

We measured particulate matter (PM) concentrations and composition at the welding teaching lab at Nueta Hidatsa Sahnish College. PM2.5 inside the welding booth ranged from 61.2-1122.6, and PM10 from 210.7-1268.4, micrograms/m^3. Outside the welding booth, PM2.5 ranged 68.7-1032.8 micrograms/m^3. ICP-MS analysis showed post air system renovation, significantly lower trace element (Pb, As, Mn, Co, Be, etc.) concentrations in the PM, and others were below detection.

Land Surface Model Impacts on the Atmosphere in the Northern Great Plains

Kaela Lucke, Aaron Scott, Aaron Kennedy, Gretchen Mullendore, University of North Dakota Atmospheric Sciences Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

This study investigates the sensitivity of a decade (2009-2018) of regional climate simulations to Land Surface Model (LSM) selection. Spin-up and microphysics parameterization tests were run to determine optimal model configuration. Results are compared to observations from the Global Historical Climatology Network (GHCN) for temperature, moisture, and precipitation. The evaluation of different LAI predictors will elucidate the impacts of a changing land surface on the atmosphere and resultant impacts on regional weather and Climate.

An Innovative Method for Estimating Planting Dates using Remotely Sensed Data

Jacob Zanker, Jon Starr, Jianglong Zhang, University of North Dakota Atmospheric Sciences Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

Accurate estimates of planting dates are crucial for crop modeling applications, yield forecasts and other agricultural applications. Using observations from the MODIS platform coupled with daily weather conditions from reanalysis data, a new method has been developed to estimate

corn planting dates at field scales (25 ha). These satellite-based planting date estimates were then inter-compared with statewide planting date statistics for North Dakota since 2003.

Development and Validation of a Library for Iterative Window-Based Processing of Geospatial Data

David Schwartz, Anne Denton, North Dakota State University Computer Science Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

With the quantity of remote sensing data available, it is imperative to develop fast algorithms to extract information. We present a Python framework that implements a set of algorithms for aggregating data within sliding windows. The algorithms have O(log(n)) time complexity and maintain the original image resolution. The framework offers several analysis methods including spectral-correlation, fractal-dimensions, slope, aspect, and curvature. We present visualizations of comparisons of multiple analyses gained using this framework.

Evaluating the Economic Trade-offs of the Devils Lake Outlet Projects

Jiyang Zhang, Afshin Shabani, Haochi Zheng, Xiaodong Zhang, University of North Dakota Earth System Science & Policy Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466, USDA AFRI

The operation of the Devils Lake outlets, a project designed to prevent future lake flooding, have caused significant increase in the salinity of Sheyenne River. This study estimates the potential damages from the increasing river salinity and compares it to the benefits from the mitigation of lake flooding. By evaluating the economic trade-offs of the outlet projects, we further discuss the optimization of regional economy and provide insights into future policymaking.

Predaceous Diving Beetle (Family Dytiscidae) Distribution Changes May Indicate Climate Change in North Dakota

Katherine Gehrig, Morgan Ohm, Andre DeLorme, Valley City State University Fisheries and Wildlife Science Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

The project goal is to establish a baseline distribution of predaceous diving beetle species across North Dakota to compare to past and future distributions. We have pulled together past data for the state, begun collecting our own adult and larval specimens, and are utilizing voucher collections from bioassessment projects dating back 20 years to pull specimens and identify to species. We hope to correlate changes in distributions with changes in climate data.

Manual Classification of Precipitation with OSCRE, the Open Snowflake Camera for Research and Education

Evan Rys, Aaron Kennedy, University of North Dakota Atmospheric Sciences Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

This project explores the feasibility of using a low-cost hydrometer camera to capture in-situ observations of wintertime precipitation. Due to the relatively low cost, the camera system has the potential to be scaled up in research departments across the country or world. In this

project, a few separate cases are explored and example hydrometoros are identified and classified manually.

Center for Sustainable Materials Science (CSMS)

UAV-Based Target-Free Structural Monitoring and Damage Identification

Mijia Yang, Xin Bai, North Dakota State University Civil and Environmental Engineering Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

Conventional vision sensors have many drawbacks, due to the motion of cameras. In this poster, the researchers will explore a recursive normalized cross correlation (NCC) method to filter out the noises due to camera's translation and rotational motions, no matter the camera's motion is induced by wind or motor engine. A series lab and field experiment are conducted to verify the concept, and excellent consistence have been reached between the input and the output.

Alternative methods to 2, 5-substituted furan diols

Catherine Sutton, Mukund P. Sibi, North Dakota State University Chemistry and Biochemistry Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

The push towards biomass-derived materials, over petroleum-derived materials, is prompted by a search for sustainability and novel chemistry. Unlike some other biomass streams, furfural production is well established.

By selectively acylating methyl-2-furoate, a furfural derivative, the potential for fine-tuned physical characteristics of the resulting materials may be realized. Results of furanic biomass valorization by acylation via green synthetic methodologies will be discussed.

Analysis of Organics and Noncondensable Gases Present in Subcritical Water-Treated Alkali Lignin

Audrey LaVallie, Jan Bilek, Keith Voeller, Anastasia Andrianova, Katherine Furey, Bin Yao, Evguenii Kozliak, Alena Kubátová, University of North Dakota Chemistry Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466, NSF Research Experience for Undergraduates under Grant No. CHE 1460825 and CHE1156584; DakotaBioCon Grant No. IIA-1330840 and IIA-1330842;

Products (organics and noncondensable gases) of subcritical water (SW) depolymerization of lignin were analyzed by thermal desorption/pyrolysis (temperature fractionation) through pyroprobe-gas chromatography-mass spectrometry and thermal carbon analysis. Oxygen content of simple SW products in the liquid fraction led to extensive gas evolution beyond 300 C during pyrolytic analysis, leading to condensed (repolymerized) compounds. However, size exclusion chromatography demonstrated MW in residue solids consistent with some breakdown compared to untreated lignin- showing less repolymerization than anticipated.

Dimerization of Biobased p-Coumaric Acid in Green Medium Using Blacklights

Briana Krupinsky, Alexandra Rios Diaz, Houssein Amjaour, Zhihan Wang, Qianli Rick Chu, University of North Dakota Chemistry Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

Biomass is a renewable feedstock that has potential for use in photochemical applications. Biomass derived *p*-coumaric acid has been utilized to form a monomer through a [2+2]

photocycloaddition after exposure to UV light. In a slurry reaction, brine has been utilized as a greener solvent alternative for the optimization of this reaction with a comparative yield and purity. This biobased photodimer has the potential to be a novel building block in green polymer synthesis.

Efficient and Direct Acetoacetylation of Lignin and Use in the Formation of Non-Isocyanate Rigid Foams

Alexander Hart, Eric Krall, Dean Webster, North Dakota State University Coatings and Polymeric Materials Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

Polyurethane polymers have become widely used in the polymer industry. Growing concern over the adverse health effects of isocyanates, a precursor to polyurethanes, has led researchers to look at alternative chemistries to generate foams. Catalyst-free valorization of lignin by transacetoacetylation was achieved in a one-pot synthesis. The acetoacetate group reacts quickly and exothermically with primary amines at room temperature. This exotherm and polysiloxane blowing agents were both used to generate rigid cellular foams.

Cyclobutanediol Derived from Biomass and Their Application in Polymer Synthesis

Rahul K. Shahni, Micah Mabin, Zhihan Wang, Muneer Shaik, Angel Ugrinov, Qianli R. Chu, University of North Dakota Chemistry Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

Semi-rigid, thermally stable, diols suitable for materials synthesis are uncommon. They bridge the gap between flexible aliphatic chain and rigid aromatic counterparts. One such example is trans-1,3-cyclobutane dimethanol (CBDO-1), which was readily synthesized from trans-cinnamic acid derived from agro-residues via [2+2] a solid-state photoreaction. A diverse array of polyesters were synthesized by polycondensation of CBDO-1 and diacids to demonstrate applications of CBDO-1 in polymer synthesis. Furthermore, these new series of polyesters showed desirable thermal properties.

Computational Determination of the Rigidity of Single Molecules

Joseph Robertson, Qianli R. Chu, University of North Dakota Chemistry Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

Rigidity of single molecules is simply described here by Eq. 1 using Van der Waals volume, VW, and two new properties, the Rigidity Factor, Rgf, and the Van der Waals potential volume, VWpot. VWpot is defined as the minimum volume occupied when all local minimum energy conformations are overlaid and aligned. Calculation of VWpot was completed using software written by the authors. Rgf may prove to be a useful tool in prediction of materials properties.

Direct Excitation to Access the Triplet State of Fumaric and Maleic Acids in the Synthesis of Cyclobutane-1,2,3,4-tetracarboxylic Acid Using ECO-UV

Dominic N. Nkemngong, Tiffany Shiu, Quintin Elliott, Rahul K. Shahni, Micah Mabin, Angel Ugrinov, Qianli Rick Chu, University of North Dakota Chemistry Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

This study presents the synthesis of cyclobutane-1,2,3,4-tetracarboxylic acid (CBTA-1). This building block is a potential useful monomer in the making of a variety of materials such as

polyamides, polyesters, and metal–organic frameworks. Two synthetic routes exhibiting a simple, efficient, and ecofriendly method were carried out without using any photocatalyst or photosensitizer. CBTA-1 was synthesized by the direct excitation of maleic and fumaric acids using germicidal lamps.

Solid-State Photoreaction to Create a Functionally Unique Two-Dimensional Polyester

Brent Kastern, Jenna Puttkammer, Rahul Shahni, Zhihan Wang, Zijun Wang, Qianli Rick Chu, Angel Ugrinov, University of North Dakota and North Dakota State University Chemistry Departments

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

This research advances the development of polymer materials that are strong and lightweight as well as being bio-based. Sorbic acid is used as the starting material for synthesizing a tetrafluorophenyl diester monomer compound. Cystallization of this compound produced an ordered arrangement of diester monomers. The reactive carbons of the diester monomers reacted in the presence of UV light and caused the diester monomers to photochemically bond with each other to produce a 2D polymer.

Wheat Bran and Maple Leaf Biochar for Decontamination of Wastewater

Creighton Pfau, Sean Pollack, Trevor Gravseth, Lexi Carpenter, Niloy Sarker, Khwaja Hossain, Mayville State University Biology Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

Dyes and toxic heavy metals are major pollutants caused by industrial run off. These pollutants negatively alter the chemical composition of water sources and have been linked to increase cancer rates, skin diseases, and slow mental development in children. Biochar, a bioproduct made from waste can be used to adsorb to these molecules. This experiment explores using spectrophotometric methods to observe pollutants before and after biochar treatment.

Lignin Solubilization and Fractionation in Aqueous Aprotic and Protic Solvents

Jessica Emond, Nafisa Bala, Bin Yao, Lindsey Bottom, Brooke Meyer, Lacy Lilleboe, Audrey LaVallie, Surojit Gupta, Evguenii Kozliak, Alena Kubatova, University of North Dakota Chemistry Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

Lignin is an organic macromolecule that is found in plant cell walls and is recovered as a large scale waste byproduct of the paper making industry. Lignin utilization often centers on its solubility and fractionation in various solvents. In this study the solubilization of Kraft alkali lignin in various organic solvents was investigated using their various ratios with water. The resulting fractions were analyzed by various analytical methods.

Comparison of Epoxidation Methods for Bio-Based Oils: Dioxirane Intermediates Generated from Oxone vs. Peracid Derived from Hydrogen Peroxide

Raul Setien, Shokoofeh Ghasemi, Ghasideh Pourhashem, Dean C. Webster, North Dakota State University Coatings and Polymeric Materials Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

Epoxidized Oils are typically synthesized using hydrogen peroxide, as well as acetic acid or other acid equivalents. Recently, advances have been made in the process of using Oxone and

ketones to generate in situ dioxiranes to epoxidize alkenes. This study explores the epoxidation of oils using in situ generated dioxiranes. The study then focused on the preparation of cured materials using said epoxidized oils as well as an environmental sustainability assessment of the oils.

Sustainability Assessment of Lignin Valorization into Rigid Foams

Ramsharan Pandey, Dean C. Webster, Ghasideh Pourhashem, North Dakota State University Coatings and Polymeric Materials Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

Lignin is the second most abundant biopolymer on earth. One potential application of lignin is in the manufacture of rigid foams. In this study we perform an economic and environmental assessment of lignin-based foam. Our results show that lignin-based foam have the potential to be economically competitive and perform environmentally better in most impact categories than rigid polyurethane foams. Functionalizing chemical and crosslinker contributed most in both economic and environmental impacts for lignin foam.

Effect of Wheat Bran Bioactive Compounds in Cancer Intervention

Brooke Roeges, Taylor Stegman, Hayle Boechler, Sean Pollack, Michael Kjelland, Khwaja Hossain, Mayville State University Biology Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

Wheat bran is rich with bioactive compounds with antioxidant properties to reduce radical oxidation that leads to malignant tumor development and growth. Bioactive chemicals such as phenolic compounds, specifically ferulic acid as well as arabinoxylan and alkyl resorcinol were extracted from wheat bran. MIA Pa-Ca2 pancreatic carcinoma cells were cultured, and concentrations of these compounds were introduced into treatment cells. These cells were compared to control cells for DNA fragmentation analysis and live to dead ratio.

Synthesis of N-[1-(4-chlorophenyl)ethyl]-N-ethylformamide

Salina R. Carter, Lioudmila I. Bobyleva, Mikhail M. Bobylev, Minot State University Chemistry Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466, NIH grant 8 P20 GM103442-12 from the National Institute of General Medical Sciences

Recently, we developed a new procedure for the synthesis of substituted N-(1-arylethyl)-N-alkylformamides. The procedure was applied to the synthesis of N-[1-(4-chlorophenyl)ethyl]-N-ethylformamide. The reaction was conducted on 10 mmol scale at 180-187 degrees Celsius. Column chromatography was used for the isolation and purification of the product. NMR-spectroscopy and elemental analysis were used to determine the structure of the product. The reaction was completed in 210 minutes. The isolated yield of N-[1-(4-chlorophenyl)ethyl]-N-ethylformamaide was 90.8%.

Rapid Synthesis of N-methyl-N-[1-(1-naphthyl)ethyl]formamide

Christopher M. Scott, Lioudmila I. Bobyleva, Mikhail M. Bobylev, Minot State University Chemistry Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466, NIH grant 8 P20 GM103442-12 from the National Institute of General Medical Sciences

Recently, we developed a new procedure for the synthesis of substituted N-(1-arylethyl)-N-alkylformamides. In this work, the procedure was applied to the synthesis of N-methyl-N-[1-(1-naphthyl)ethyl]formamide. The reaction was conducted on 10 mmol scale at 196-202 degrees Celsius. Column chromatography was used for the isolation of the product. NMR-spectroscopy and elemental analysis were used to determine the structure of the product. The reaction was completed in 40 minutes. The isolated yield of N-methyl-N[1-(1-naphthyl)ethyl]formamide was 94.5%

Synthesis of N-[1-(4-cyanophenyl)ethyl]formamide

Hassan S. Elshanbary, Lioudmila I. Bobyleva, MS, Mikhail M. Bobylev, Minot State University Bio-informatics Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466, NIH grant 8 P20 GM103442-12 from the National Institute of General Medical Sciences

Recently, we developed a new procedure for the synthesis of substituted N-(1-arylethyl)formamides. In this work, the procedure was applied to the synthesis of N-[1-(4-cyanophenyl)ethyl]formamide. The reaction was conducted on 10 mmol scale at 180-193 degrees Celsius. Column chromatography was used for the isolation of the product. NMR-spectroscopy and elemental analysis were used to determine the structure of the product. The reaction was completed in 10 minutes. The isolated yield of N-ethyl-N-[1-(4-isobutylphenyl)ethyl]formamide was 74.7%.

Rapid Synthesis of N-[1-(4-nitrophenyl)ethyl]formamide

Lynn I. Vick, Lioudmila I. Bobyleva, MS, Mikhail M. Bobylev, Minot State University Biology Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466, NIH grant 8 P20 GM103442-12 from the National Institute of General Medical Sciences

Recently, we developed a new procedure for the synthesis of substituted N-1-(arylethyl)formamides. In this work, the procedure was applied to the synthesis of N-[1-(4-nitrophenyl)ethyl]formamide. The reaction was conducted on 10 mmol scale at 180-191 degrees Celsius. Column chromatography was used for the isolation of the product. NMR-spectroscopy and elemental analysis were used to determine the structure of the product. The reaction was completed in 5 minutes. The isolated yield of N-[1-(4-nitrophenyl)ethyl]formamide was 74.6%.

Synthesizing Various Ruthenium Complexes for C-H Bond Hydroxylation

Austin MacRae, Alexander Parent, North Dakota State University Chemistry and Biochemistry Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

Metal complexes can catalyze C-H bond hydroxylation, which is potentially useful in the synthesis of organic molecules such as pharmaceutical drugs. Current catalysts suffer from the sustainability drawbacks of overoxidation and racemization. A catalyst that favors a two-electron catalytic process may overcome the issues of overoxidation and racemization by insertion of an oxygen atom into the C-H bond. Ruthenium complexes with varying anionic ligands will be characterized for their electrochemical properties and catalytic capabilities.

Biobased Latexes from 3-Allyl-5-vinylveratrole and High Oleic Soybean Oil-based Acrylic Monomer

Yehor Polunin, Eric Serum, Timothy Burns, Andriy Voronov, Mukund Sibi, North Dakota State University Coatings and Polymeric Materials Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

Being structural analog to Styrene, vanillin derived 3-allyl-5vinylveratrole may function as its renewable replacement in free radical polymerization, in particular in sustainable latexes. AVV was applied as a comonomer in latex copolymerization with plant oil-based acrylic monomers (POBMs). Presence of AVV fragments increase glass transition temperature of latex copolymers and provides crosslinking sites in addition to allylic fatty fragments of POBMs. Depending monomers ratio, polymeric materials with widely different viscoelastic behavior were obtained.

Molecular Dynamics Study of Invertible Micellar Polymer Assemblies in Toluene

Kweeni Iduoku, Rasulev Bakhtiyor, North Dakota State University Coatings and Polymeric Materials Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

Invertible micellar polymer assemblies are amphiphilic in nature and are capable of changing their conformation in response to environmental stimuli. This characteristic is a result of systematic arrangements of moieties and segments along the backbone of polymer chain. In the solvent toluene, there is a migration of hydrophobic segments to micellar peripheral and hydrophilic segments to core. Molecular dynamic has been employed to unveil the molecular and atomistic properties of micellar assemblies in toluene.

Data Collection of Organic Compounds for Predictive Model Development of Biodegradability Applying Various Cheminformatic Techniques

Marvellous Ngongang, Meade Erickson, Bakhtiyor Rasulev, North Dakota State University Coatings and Polymeric Materials Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466, The State of North Dakota

Readily biodegradable materials are of increasing importance due to regulatory institutions increasing regulations and guidances of chemical materials. The ability to predict the biodegradability of chemicals is an effective method in developing readily biodegradable chemicals. In this study, the predictive computational techniques are used to develop readily biodegradable models to be able to asses biodegradation in advance of synthesis of manufacturing. The results and comparative analysis of different methods performance are discussed.

Brine Spill Remediation Using Natural Fiber Wicks

Jake Reinholz, Tom DeSutter, Chad Ulven, Miranda Meehan, Kevin Horsager, North Dakota State University Mechanical Engineering Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466, USDA-Critical Agriculture Research and Extension

Brine, or high salt-concentrated water, is a byproduct of oil and natural gas production. In the Bakken Shale of North Dakota, brine spills leave fertile land virtually unusable. The goal of this research is to create a remediation technique using natural fiber mats to act as an evaporative

flux that wicks brine from the soil. As brine water evaporates, harmful salts remain integrated within the mat fibers which can then be collected and disposed.

Predicting the Biodegradability of Synthetic and Bio-based Polymer Building Blocks: Collection of Biochemical Oxygen Demand and Application of Cheminformatics

Meade Erickson, Zoriana Demchuk, A.N. Bezbaruah, Andriy Voronov, Bakhtiyor Rasulev, North Dakota State University Coatings and Polymeric Materials Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466, ND Soybean Council, ND Corn Council, ND Department of Agriculture, the State of North Dakota

Polymeric waste is accumulating in varying environments globally. This is a result of the low degradability of polymers. A method of addressing this waste is to develop biodegradable materials. This research focuses on biodegradation study, by investigating monomer units' molecular structure and its relationship with biodegradability. Using combined experimental and computational study, applying machine learning-based quantitative structure-activity relationship (QSAR) methodology, a predictive model has been developed.

Rapid Synthesis of N-(4-nitrobenzyl)-N-phenylformamide

Taylor L. Simons, Lioudmila I. Bobyleva, Mikhail M. Bobylev, Minot State University Chemistry Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466, NIH grant 8 P20 GM103442-12 from the National Institute of General Medical Sciences

Recently, we developed a rapid procedure for the synthesis of substituted N-benzyl-N-arylformamides. The procedure was tested on 4-nitrobenzaldehyde. The reaction was conducted on 10 mmol scale at 173-225 degrees Celsius. Column chromatography was used for the isolation the products. NMR-spectroscopy and elemental analysis were used to determine the structure of the products. The reaction was completed in 17 minutes and produced 49.9% N-(4-nitrobenzyl)-N-phenylformamide and 38.8% of N,N-di-(4-nitrobenzyl)-N-phenylamine.

Developing a Vesicle System for Efficient Solar Energy Conversion

Adam Flesche, Andrew Kalbach, Alexander Parent, North Dakota State University Chemistry Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

Harvesting light for use in energy production is a promising approach towards limiting the use of non-sustainable fuel sources. One major challenge in developing this technology is charge recombination, where the absorbed light is released as heat before it can be converted to a useful energy source. This may be remedied by separating the half-reactions with a physical barrier. Our group is developing a soft vesicle system to prevent charge recombination.

Rapid Synthesis of N-[1-(2,4-dichlorophenyl)ethyl]-N-ethylformamide

Micah S. Winburn, Lioudmila I. Bobyleva, Mikhail M. Bobylev, Minot State University Chemistry DepartmenT

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466, NH grant 8 GM103442-12 from the National Institute of General Medical Sciences

Recently, we developed a new procedure for the synthesis of substituted N-benzyl-N-

alkylformamides. In this work, this procedure was applied to the synthesis of N-[1-(2,4-dichlorophenyl)ethyl]-N-ethylformamide. The reaction was conducted on 10 mmol scale at 180-196 degrees Celsius. Column chromatography was used for the isolation of the product. The stucture was determined using NMR-spectroscopy and elemental analysis. The reaction was completed in 210 minutes. The isolated yield of N-[1-(2,4-dichlorophenyl)ethyl]-N-ethylformamide was 70.1%.

Protein-ligand Docking as a Tool to Predict Properties and Performance of Plant-protein Based Bioplastics Films

Kristen Patnode, Sara Johnson, Zoriana Demchuk, Andriy Voronov, Bakhtiyor Rasulev, North Dakota State University Coatings and Polymeric Materials Department

Sponsor: ND EPSCoR, North Dakota Soybean Council, North Dakota Corn Utilization Council

The aim of this study is to determine the efficacy of protein-ligand docking as a means to estimate physical and mechanical properties of modified bioplastics. Protein-ligand docking was applied to model intermolecular interactions of select renewable additives with plant proteins, to demonstrate the effect of natural modifiers on properties of protein-based films. We support computational findings via experimental preparation of modified soy and Zein protein-based films. Results demonstrate successful estimation of properties via protein-ligand docking.

Chemistry

Fe3+ - doped Graphene Quantum Dots for Ultrasensitive Detection of Glucose and Monitoring of Diabetes

Yingfen Wu, Xu Wu, Julia Xiaojun Zhao, Diane Darland, University of North Dakota Chemistry Department

Sponsor: NSF grant CHE 1709160 and NSF Cooperative Agreement Award OIA-1946202. D.C.D. is supported by an NIH COBRE grant as Project Director

Test the blood glucose concentration is of great importance for patients with diabetes or related diseases. In this paper, a new graphene quantum dots (GQDs-Fe) were successfully synthesized with Fe(III) ion and hydrophilic polyethylenimine (PEI)to detect H2O2 and glucose. The morphology, properties, and potential of detection were determined by analytical spectroscopy methods. The newly synthesized GQDs show high potential for its application in H2O2 and glucose detection.

Development of Polymer Dot @ Silicon Quantum Dots Nanocomposite for Fluorescence Imaging

Di Sun, Xu Wu, Diane C. Darland, Julia Xiaojun Zhao, University of North Dakota Chemistry Department

Sponsor: NSF EPSCoR

Silicon Quantum dots (SiQDs) have been widely developed in recent years. However, SiQDs are very unstable and are susceptible to aggregation, which would reduce quantum yield (QY). We constructed a Pdot@SiQDs nanocomposite by using amine group terminated SiQDs and carboxyl group terminated Pdots-PVK. In the nanocomposite, the Forster resonance energy transfer (FRET) occurred where the Pdots was used as an energy donor to excite SiQDs to emit strong fluorescence and prevent aggregation of SiQDs.

Poly(silyl ether)-based Polymeric Nanoparticles as Potential Nanocarriers

Vladimir Zotov, Guodong Du, University of North Dakota Chemistry Department

Sponsor: UND, ND EPSCoR, NSF EPSCoR RII Track-1

Polymeric nanoparticles are currently a widely studied topic due to their potential in therapeutics of different diseases. Poly(silyl ether) (PSE) based polymers are of interest due to their tunable hydrolytic degradability. PSE formation occurs between a disubstituted silane and a diol via dehydrogenate cross coupling reactions. To modify the degradation of PSEs under physiologically relevant conditions, polyethylene glycol (PEG) based diols have been employed to prepare PSEs, which will be used in formation of nanoparticles.

New Cyclobutane Containing Polyesters from Zinc Catalyzed Ring-opening Copolymerization of Epoxides and Cyclobutane-based Anhydrides

Muneer Shaik, Jevin Jensen, Houssein Amjaour, Qianli Chu, Guodong Du, University of North Dakota Chemistry Department

Sponsor: NSF EPSCoR

Aliphatic polyesters have received attention as attractive and potentially sustainable alternatives to petroleum-based polymers due to their various renewable sources, degradation to usually benign products, and high biocompatibility. In this work, we have synthesized a series of new polyesters via zinc-catalyzed ring-opening copolymerization of epoxides and novel cyclobutane-derived anhydrides. The polymers have been characterized by NMR, DOSY, ESI, GPC, TGA, and DSC.

Sustainability and Techno-Economic Assessment of Expoxidized Sucrose Soyate

Shokoofeh Ghasemi, Mukund Sibi, Dean C. Webster, Ghasideh Pourhashem, North Dakota State University Coatings and Polymeric Materials Department

Sponsor: NSF EPSCoR

We carried out a comparative life cycle assessment (LCA) of Epoxidized Sucrose Soyate (ESS) and a functionally similar petroleum-based commercial resin. We model the large-scale production of ESS using laboratory-scale experimental data using Aspen plus software and use the results to assess the sustainability and cost of producing ESS resin on a commercial scale. To assess the economic feasibility of production of ESS commercially, we perform techno-economic analysis (TEA) to provide critical decision-making information.

Improving Pea Protein Isolate Functionality by Phosphorylation with Sodium Hexametaphosphate

Yang Lan, Jiajia Rao, North Dakota State University Chemistry Department

Sponsor: None

Pea protein isolate (PPI) is commonly extracted using the method of alkaline extraction-isoelectric precipitation, followed by spray drying process; however, PPI prepared from this procedure has limited functionality. This study investigated the phosphorylation modification of PPI and the impact of sodium hexametaphosphate-PPI mixing ratios and reaction pH on PPI structure and functionality. Results showed that PPI has been successfully phosphorylated and foaming capacity of PPI has been improved from 110 to 120%.

Synthesis and Properties of Cyclobutene-containing Anhydrides

Houssein Amjaour, Rahul K. Shahni, Mckenzie Roman, Zhihan Wang, Angel Ugrinov, Qianli R. Chu, University of North Dakota Chemistry Department

Sponsor: NSF EPSCoR

Anhydrides are important intermediates employed in the manufacture of a variety of materials such as fiber-reinforced plastics, surface coatings, polyimides and agricultural chemicals. Herein, we report the synthesis and properties of series of cyclobutane-containing anhydrides. Some of the anhydrides were readily synthesized from biomass-derived chemicals such as furfural. These anhydrides showed an excellent balance between stability and reactivity due to the ring strain generated by cyclobutane fused to the cyclic anhydride functional group.

Hypoxia-Responsive Bovine Milk Exosomes as Targeted Carrier for Chemotherapeutics

Jessica Pullan, Li Feng, Kaitlin Dailey, Sangeeta Bhallamudi, James Froberg, Lina Alhalhooly, Amanda Brooks, Sathish Venkatachalem, Yongki Choi, Sanku Mallik, North Dakota State University Pharmaceutical Sciences Department

Sponsor: NIH

Exosomes, biological nanoparticles, have innate transportation ability making them ideal candidates for drug delivery. Bovine milk exosomes do not show an immune response and is available from a viable source. To increase targeting and controlled drug release, a tumor penetrating peptide (iRGD) and a hypoxia-responsive lipid have been incorporated into the exosomes' lipid bilayer. Modified exosomes encapsulating doxorubicin decreased the viability of triple negative breast cancer cells.

Synthesis of N-N'-dimethyl-N,N'-(1,4-phenylenediethylidene)bis-formamide

Stephanie E. Sundhagen, Isabella Rowland, Lioudmila I. Bobyleva, Mikhail M. Bobylev Minot State University Chemistry Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-

1355466, NIH grant 8 P20 GM103442-12 from the National Institute of General Medical Sciences

Recently, we developed a new procedure for the synthesis of substituted N-(1-arylethyl)-N-alkylformamides. In this work, the procedure was applied to the synthesis of N,N'-dimethyl-N,N'-(1,4-phenylenediethylidene)bis-formamide. The reaction was conducted on 10 mmol scale at 185-187 degrees Celsius. Column chromatography was used for the isolation of the product. NMR-spectroscopy and elemental analysis were used to determine the structure of the product. The reaction was completed in 20 minutes. The isolated yield was 76.8%.

A FRET Ratiometric Nanohybrid Assembly with Gold Nanoclusters and Conjugated Polymers Nanoparticles for Cysteine Detection

Hannah Juan Han, Julia Xiaojun Zhao, David T. Pierce, University of North Dakota Chemistry Analytical Chemistry Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

We have developed a nanohybrid using gold nanoclusters (AuNCs) and polyvinylcarbazole polymer nanoparticles (PVK PNs) that demonstrated strong fluorescence resonance energy transfer (FRET). Fluorescence quantum yield of AuNCs enhanced from 1 % to 3% through FRET. Fluorescence lifetime measurements indicate a 59 % FRET efficiency. Fluorescent nanohybrid is sensitive to cysteine through a quenching process and can be used to determine cysteine from 0.5 to 600 uM with LOD of 0.18 uM.

Rapid Synthesis of N-[1-(4-biphenyl)ethyl]-N-methylformamide

Aziza Z. Ziiadinova, Lioudmila I. Bobyleva, Mikhail M. Bobylev, Minot State University Biology Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466, NIH grant 8 P20 GM103442-12 from the National Institute of General Medical Sciences

Recently, we developed a new procedure for the synthesis of substituted N-(1-arylethyl)-N-alkylformamides. In this work, the procedure was applied to the synthesis of N-[1-(4-biphenyl)ethyl]-N-methylformamide. The reaction was conducted on 10 mmol scale at 196-200 degrees Celsius. Crystallization was used for the isolation of the product. NMR-spectroscopy and elemental analysis were used to determine the structure of the product. The reaction was completed in 30 minutes. The isolated yield of N-[1-(4-biphenyl)ethyl]-N-methylformamide was 87.4%.

Synthesis of N-ethyl-N-[1-(4-isobutylphenyl)ethyl]formamide

Daniela Nardelli, Lioudmila I. Bobyleva, Mikhail M. Bobylev, Minot State University Biology Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466, NIH grant 8 P20 GM103442-12 from the National Institute of General Medical Sciences

Recently, we developed a new procedure for the synthesis of substituted N-(1-arylethyl)-N-alkylformamide. In this work, the procedure was applied to the synthesis of N-ethyl-N-[1-(4-isobutylphenyl)ethyl]formamide. The reaction was conducted on 10 mmol scale at 186-196 degrees Celsius. Column chromatography was used for the isolation of the product. NMR-spectroscopy and elemental anysis were used to determine the structure of the product. The

reaction was completed in 100 minutes. The isolated yield of N-ethyl-N-[1-(4-isobutylphenyl)ethyl]formamide was 87.4%.

Synthesis of Hypoxia-Responsive Block Copolymers

Li Feng, Sanku Mallik, North Dakota State University Pharmaceutical Department

Sponsor: None

Hypoxia occurs in solid tumors because of inadequate blood supply. In this study, we synthesized a series of hypoxia responsive diblock copolymers poly(lactic acid)-azobenzene-poly(ethylene glycol) with different molecular weights and hypoxia sensitive units. The synthesized copolymers self-assemble to form polymersomes in aqueous media. We demonstrated the efficient release of encapsulated anticancer drugs from the polymersomes under hypoxia conditions in pancreatic and triple-negative breast cancer cells.

Adsorption and reaction of sulfur compounds on graphene at ultra-high vacuum – a surface science study

Thomas Stach, Melody C. Johnson, Samuel Stevens, Uwe Burghaus, North Dakota State University Department of Chemistry and Biochemistry

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466

Noble metal-free catalysis using functionalized carbon is an emerging alternative to traditional chemical synthesis. Examples are known for liquid phase and gas-phase reactions. In particular, reactivity towards adsorption/reaction of sulfur compounds has been demonstrated in the literature. However, gas-surface reactions are not well studied. Our first results using kinetics techniques and spectroscopy indeed show that SO2 and H2S dissociate on graphene epitaxially grown on ruthenium. Further experiments will reveal a detailed reaction mechanism.

Computer and Information Science and Engineering

Synthesis and Properties of Cyclobutane-containing Anhydrides

Houssein Amjaour, Rahul K. Shahni, Mckenzie Roman, Zhihan Wang, Angel Ugrinov, Qianli R. Chu, University of North Dakota Chemistry Department

Sponsor: None

Anhydrides are important intermediates employed in the manufacturing of a variety of materials such as fiber-reinforced plastics, surface coatings, polyimides, and agricultural chemicals. Herein, we report the synthesis and properties of series of cyclobutane-containing anhydrides. Some of the anhydrides were readily synthesized from biomass-derived chemicals such as furfural. These anhydrides showed an excellent balance between stability and reactivity due to the ring strain generated by a fusion of cyclobutane to the cyclic anhydride functional group.

Engineering

Development of Synchronous and Asynchronous Interactive Virtual Lab Modules for Thermal Systems Laboratory at NDSU

Yan Zhang, Derek Heinis, North Dakota State University, Mechanical Engineering Department

Sponsor: ND EPSCoR

The COVID-19 pandemic poses significant challenges to engineering lab education. To better accommodate the needs of enhanced virtual lab learning, we improved the NDSU ME457 Thermal Systems Lab course with innovative virtual lab modules. The synchronous component is made possible through live broadcastings of physical experiments using tablet computers. The asynchronous component is achieved by interactive modules of simulated labs. This virtual lab enables a HyFlex delivery mode of ME457 for the first time.

Analyzing the Environmental and Economic Benefits of Establishing a Centralized Construction and Demolition Waste Recycling Facility in North Dakota

Simon Boateng, Abdul-Aziz Banawi, North Dakota State University, Construction Management Department

Sponsor: ND EPSCoR

The purpose of this study is to apply Life Cycle Assessment and Life Cycle Cost in evaluating the benefits of establishing a construction and demolition waste (CDW) recycling facility. preliminary findings from this ongoing study revealed that recycling CDW in Fargo has environmental benefits of reducing carbon footprint by 47Co2 eq. kg/ton of CDW while generating a revenue of 29.85/ton for the city.

Biosensing Environment for Responses to Built Environments

Ganapathy Mahalingam, Sydney Garcia and Jenna Bordwell, North Dakota State University, Architecture Department

Sponsor: ND- EPSCoR (NDSU STEM Research and Education Program 2019)

The funding received from ND-EPSCoR was used to acquire research infrastructure to enable research studies in the biosensing of the built environment. Two types of biosensing equipment were acquired: a set of components that made up a BCI (brain computer interface) and a set of wearable sensors that would track the vital signs of building users. Two research studies were conducted using part of the equipment to test their deployment. The results are presented.

Surface Thermodynamic Properties of Per- and Polyfluoroalkyl Substances (PFAS) Aerosols

Hallie Boyer Chelmo, Sidney Arbogast, Emily Dahlke, Bryan Kovacic, Gabriel Schettler, Fafa Tackie-Otoo, Taylor Strand, Logan Webber, Feng Xiao, University of North Dakota Mechanical Engineering Department

Sponsor: None

A custom aerosol optical tweezers traps PFAS aerosols, while controlling temperature and humidity, and measures size, concentration, surface tension, and pH. All of these properties feedback on each other and require this in situ technique to directly probe individual droplets while keeping the surface pristine and unperturbed. For the surface tension model, parameters were reduced through dependence on the critical micelle concentrations of various PFAS compounds.

Destruction of "Forever" Chemicals

Pavankumar Challa Sasi, Ali Alinezhad, Bin Yao, Alena Kubatova, Svetlana A. Golovko, Mikhail Y. Golovko, Feng Xiao, University of North Dakota Civil Engineering Department

Sponsor: EPA

The aims of these studies were twofold, to improve our understanding of thermal decomposition behaviors of per- and polyfluoroalkyl substances (PFAS) and to investigate the decomposition of these compounds on spent granular activated carbon (GAC) during GAC thermal reactivation. Our results showed that decomposition of PFCAs initiated at temperatures as low as 200 C and >450 C for PFSAs. Achieved near complete (>99.9%) decomposition of PFOA and PFOS at >700 C.

Effects of Biochar on the Loss of Nutrients from Soil

Swetha Mallula, Advisor: Dr. Xiao Feng, University of North Dakota Civil Engineering Department

Sponsor: None

We investigated the growth of soybean and loss of nutrients from soil with the addition of raw and thermally air oxidized biochars produced at different temperatures and applied at different application rates. Concentrations of nitrate, phosphorous, and ammonia were measured in the leachate from the biochar-amended soil with or without fertilizer. This research enhances our understanding of the impact of biochar amendment on crop growth and the fate of nutrients in agricultural soil.

Adsorption and Thermal Decomposition of Per- and Polyfluoroalkyl Substances (PFAS) and PFAS Alternatives in Soil from Landfill Leachate

Ali Alinezhad, Pavankumar Challa Sasi, Feng Xiao, University of North Dakota Environmental Engineering Department

Sponsor:

Per- and polyfluoroalkyl substances (PFAS) are organic compounds used in various industrial and commercial applications. A major course of contamination of PFAS in soil and groundwater is the landfill leachate. In this study, adsorption of PFAS to soil from landfill leachate and thermal decomposition of PFAS in soil were studied. We found that PFAS can be effectively degraded at 400 oC and above. Methanol amended with ammonium acetate can effectively extract PFAS from soil samples. The thermal decomposition of perfluoroalkyl carboxyl acids (PFCAs) was little affected by the initial loading of PFCA to soil/clay. On the other hand, perfluoroalkyl sulfonic acids (PFSAs) required a much higher temperature to decompose, which was affected greatly by the initial loading of PFSA to soil/clay at temperatures at which PFSAs partially decomposed.

Memristor Based Noise Injection of Differential Privacy for Neuromorphic Computing

Jingyan Fu, Zhiheng Liao, Jianqing Liu, Scott C. Smith, Jinhui Wang, North Dakota State University Electrical and Computer Engineering Department

Sponsor: NSF EPSCoR Track-1

We propose a Noise Distribution Normalization method to add Gaussian distributed noise through the hardware implementation, thereby achieving differential privacy in edge AI. Instead of using traditional algorithmic noise-insertion methods, we take advantage of inherent cycle-to-cycle variations of memristors during the weight-update process as the noise source, which does not incur extra software or hardware overhead.

Detection of Prostrate Specific Antigen Using a Bioelectronic Sensor

Fleming Dackson Gudagunti, Srilakshmi Gundlakunta, Dharmakeerthi Nawarathna, Ivan T. Lima Jr., North Dakota State University Electrical and Computer Engineering Department

Sponsor: None

Early detection of prostate cancer (PCa) is an important medical tool as PCa causes an average of 307,000 annual related deaths worldwide. Prostate-specific antigen (PSA) is a protein made by the prostate gland that is an effective biomarker of PCa. In this study, we demonstrate that dielectrophoresis spectroscopy is an effective label-free transduction mechanism for the detection of the cutoff levels of PSA that are relevant in the diagnosis of PCA.

Mechanical Behavior and Deformation Mechanism of Conjugated Polymer via Molecular Dynamics

Amirhadi Alesadi, Wenjie Xia, North Dakota State University Civil Engineering Department

Sponsor: ND EPSCoR

Understanding the mechanical behavior of conjugated polymers at the fundamental molecular level is important in various engineering applications. In this study, we employed molecular dynamics (MD) simulations to study the influence of side-chain groups on the deformation mechanism and glass transition of conjugated polymers. The results indicated that MD simulations are able to capture the physical behavior of these semiconducting polymers, and can validate the relevant experimental data.

Coal-derived Graphene as a 3D Free-standing Lithium-ion Battery Anode

Xin Zhang, Xiaodong Hou, Michael Mann, University of North Dakota Institute for Energy Studies

Sponsor: NSF EPSCoR

The use of graphene for porous 3D anodes for Lithium-ion battery is a promising route due to its designable single sheet-like structure, excellent electrical conductivity, high surface area. This study investigated the feasibility of the freestanding Si@G foam anode using coal-derived graphene. The Silicon particles were loaded on the graphene skeleton properly to form the freestanding Si@G foam which exhibits stable electrochemical performance of high specific capacity, cycling stability, and good rate performance.

A Blockchain Based IoT Framework for Oil and Gas Industry Remote Control, Predictive Maintenance and Automation and Control

Zhenyu Qi, Yanjun Zuo, Hui Pu, Joseph Lindemann, University of North Dakota Accountancy Department

Sponsor: ND EPSCoR

The Internet of Things (IoT) is a transformative technology to enable seamless real-time data collection, remote control, and predictive maintenance of equipment, processes, and operations in the Oil and Gas industry. In this study, we propose a blockchain-based IoT framework to deliver automatic, decentralized and trustworthy services to increase operational and asset efficiency and safety of oil and gas operations. We present the key components of the framework including system architecture, algorithms, and smart contracts.

Bio-based Coating for Mitigating Corrosion in Rebars

Hizb Ullah Sajid, Ravi Kiran Yellavajjala, North Dakota State University Civil and Environmental Engineering Department

Sponsor: MN Soybean Research & Promotion Council

Corrosion is widely recognized as a major deterioration mechanism in reinforced concrete structures. This study aims at synthesizing and characterizing the performance of a new soy-based coating material for mitigating corrosion in rebars. To this end, the physical and chemical characteristics of the coating material are evaluated and the corrosion performance of the cement mortar-embedded coated rebars is investigated. The results demonstrate that the new coating material has the potential to mitigate rebar corrosion.

Geosciences

Road Ditches and Pollinator Habitat

Yeqian Xu, University of North Dakota ESSP Department

Sponsor: ND EPSCoR, UND ESSP

Pollinators play a vital role in pollination, which brings an essential benefit to ecosystem services. In this project, we study the impact and economic feasibility of road ditch serving as pollinator habitat, compared to other public-funded pollinator conservation programs. The study is employed fieldwork, geospatial analysis, and economic valuation techniques to provide policy-makers useful information to better support pollinator habitat in this region.

Life Sciences

Cultivating STEM Career Interest in North Dakota Middle School Students with Unmanned Aircraft Systems (UAS)

Woei Hung, University of North Dakota Department of Education, Health & Behavior Studies

Sponsor: ND EPSCoR

The goal of this project is to introduce Unmanned Aircraft Systems (UAS) to North Dakota middle school students to cultivate their STEM career interests. This project is to support Strategy 1 -- Technology and Unmanned Aerial Systems. Problem-based learning would be used to engage the middle school students in using UAS to solve real life problems and spark their interest in STEM and help them see potential career pathways into the UAS industry.

Mitochondrial Genome Sequencing of the Caucasian Neanderthals

Igor Ovchinnikov, University of North Dakota Biology Department

Sponsor: ND EPSCoR

Neanderthals from the Caucasus may have represented the most genetically diverse group of Neanderthals among all studied to date. To test the hypothesis about higher genetic diversity in the Caucasian Neanderthals, I first generated genome libraries from single-stranded DNA isolated from the hominin teeth excavated in Barakaevskaya and Monasheskaya caves using uracil-tolerant and uracil-nontolerant polymerases. The genome libraries will be high-throughput sequenced after the target enrichment with RNA-baits for hominin mitochondrial DNA molecules.

Airborne Cognitive State Monitoring

Nicholas Wilson, Hamed Taheri Gorji, Jessica VanBree, Bradley Hoffmann, Kouhyar Tavakolian, Thomas Petros, University and Department

Sponsor: ND EPSCoR STEM grant, John D. Odegard School of Aerospace Sciences Seed Grant

This study sought to further our understanding of pilot (N=10) cognitive state during unique flight maneuvers. Researchers collected physiological measures from pilot participants such as electroencephalogram (EEG) and combined with aircraft flight data from onboard avionics. Using EEG analytic techniques, researchers are able to show differentiation of pilot mental workload during unique flight maneuvers. These results will serve to improve our understanding of cognitive workload and offer possibilities for future research into flight safety.

Effects of 2D vs. 3D cell culture on the Epithelial-Mesenchymal Transition (EMT)

Carson Herbert, Kole Hermanson, Diane Darland, Archana Dhasarathy, University of North Dakota Biology Department and School of Medicine and Health Services

Sponsor: ND EPSCoR URA

Relative to 2D cell culture, growing breast cancer cells in 3D culture and co-culture systems have been found to more closely mimic characteristics of tumors, including cellular morphology, gene expression, splicing, and 3D chromatin structure. The goal of our project is to assess how cell growth in 2D vs. 3D affects the epithelial-mesenchymal transition (EMT), a key process involved in cancer metastasis and drug resistance.

Influence of the provision microbiome on the development of Megachile rotundata

Gagandeep S. Brar, Madison Floden. George D. Yocum, Julia H. Bowsher, North Dakota State University and Biological Sciences Department

Sponsor: NSF RII Track-2 FEC 1826834

Megachile rotundata is an important field crop pollinator. The females provision its offspring with pollen having diverse community of microbiomes that contribute to the health and survival. Evidence concerning the effects of provision microbiomes on physiology is lacking in M.rotundata. We tested the hypothesis that provision microbiome affects bee's development and survival by manipulating natural diet with diet containing antibiotics that showed significant effects on growth rate, larval, prepupal, and cocoon weight and survival.

Investigating the Diapause and Pollen Ball Incidence Dynamics in the Alfalfa Leafcutting Bee, Megachile Rotundata

Preetpal Singh, Gagandeep Singh Brar, Bridger Scrapper, Madison Floden, Joseph Rinehart, Julia Bowsher, North Dakota State University Biological Sciences Department

Sponsor: NSF RII Track-2 FEC 1826834

Megachile rotundata, is a commercial solitary pollinator of alfalfa. Cues regulating the diapause incidence and factors affecting the pollen ball incidence are not entirely understood in M. rotundata. To determine the effects of temperature, photoperiod, cell position, and population density on diapause and pollen ball incidence, we designed and installed six replicate nest boxes in alfalfa fields. Our results indicate that maternal influence played an important role in determining diapause and pollen ball incidence.

Splenectomy Ameliorates Neuroinflammation in Alzheimer's Disease Mice

Nelofar Nargis, Bijayani Sahu, Colin Combs, University of North Dakota Biomedical Sciences Department

Sponsor: None

Alzheimer's disease (AD) is characterized by neurodegeneration and dementia. Numerous studies support an immune contribution to disease progression. We hypothesized that spleen-brain communication might explain this inflammatory pathophysiology. Immunohistochemistry was performed on brains of healthy and AppNL-G-F (AD) mice to quantify phenotypes of the brain immune cell, microglia. Splenectomy decreased the inflammatory environment of AppNL-G-F brains by increasing TREM2 expressing microglia. These data confirm that peripheral immune cells contribute to brain inflammation during disease.

Pancreatic Tumor-associated Pericyte Phenotype and Function are Greatly Influenced by Tumor Microenvironment (TME)

Vikneshwari Natarajan, Alexander Delgado, Reed Jacobson, Maryam Al-Kaabi, Sangdeuk Ha, Jiha Kim, North Dakota State University Biological Sciences Department

Sponsor: NIH COBRE 1P20GM109024

Pancreatic tumor vessels display atypical characteristics causing poor perfusion, hypoxic and immunosuppressive TME, and metastasis. Our recent work indicates that tumor-associated pericytes express ectopic alpha-smooth muscle actin (a-SMA), contributing to changes in pericyte morphology, biomechanical properties, association with vessels, and overall vascular functionality. Interestingly, such aberrant phenotype was induced by cancer cell-derived exosomes. Our foundational work will help understand the importance of pericyte phenotype and develop innovative ways to re-functionalize abnormal vessels.

Synergistic Effects of All-trans Retinoic Acid (ATRA) on Triple Negative Breast Cancer Cells

Madison Koppelman, Jacob Shreffler, Sanku Mallik, North Dakota State University Pharmaceutical Sciences Department

Sponsor: EPSCoR

Triple-negative breast cancer (TNBC) is the deadliest breast malignancy and comprises 10-15% of cases. Solid tumors develop early and harbor drug-resistant cancer stem cells (CSC). All-trans Retinoic Acid (ATRA) induces differentiation of CSC in a variety of solid tumors. Herein, we demonstrate the synergistic effect of Doxorubicin and ATRA on cytotoxicity of TNBC cells in a monolayer and describe the methods of ATRA quantifications by High-performance Liquid Chromatography (HPLC).

Bladder Cancer Risk Prediction Model for Human Exposed to Arsenic: Gene Expression Analysis

Sonalika Singhal, Nathan Rupercht, Kouhyar Tavakolian, Donald Sens, Seema Somji, Scott Garrett, Sandeep Singhal, University of North Dakota Pathology Department

Sponsor: NIH: ND INBRE IDeA program P20 GM103442, DeA DaCCoTA CTR program, U54GM128729

IARC classified Arsenic (As) as "carcinogenic to humans", but despite the health consequences, there is no molecular signature available yet to predict when exposure may lead to the disease development. The aim of this study is to investigate the genetic changes due to the exposure carcinogenic compounds As using human genetics profiles. Additionally, we developed a bladder cancer predictive model that would be very helpful to forecast the outcome of As exposed in humans.

Data Driven Dynamics in Smart Connected Systems for Obstructive Sleep Apnea (OSA) Diagnosis and Treatment

Trung (Tim) Le, North Dakota State University Industrial and Manufacturing Engineering/Biomedical Engineering Department

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

Advancements in computing and sensing technologies in healthcare have yielded the largest-ever stream of data. Although our understanding of human biological processes has evolved considerably over the past few decades, unraveling the complex relationships of measured data and the underlying mechanisms of these processes pose daunting challenges due to the inherently stochastic and nonlinear attributes of biological processes. To address these challenges, this research, rooted in sensor-based modeling and nonlinear stochastic dynamic systems principles, investigates a framework for personalized prognostics of obstructive sleep apnea (OSA) in the emerging smart and connected health contexts. Such framework consists of 1) Data-driven and sensor-based modeling method to characterize the coupling dynamics of the pathological processes via investigating the nonlinear lump parameter model of the biological processes driven by the collected sensor data; 2) Design of customized IoT sensing systems that can effectively capture the signals of interest for the extraction of characteristic features in enriched domain notwithstanding the constraints from current clinical needs and 3) Predictive analytics approach to forecast acute event onsets by qualifying the transition of the system dynamics from the normal to abnormal conditions for personalized prognostic healthcare. The proposed approaches have been evaluated from in-vitro, and in-vivo to human subject models.

Novel Breath Acetone Sensor Based on 1D/2D Nanocomposite for Diabetes Prevention and Monitoring

Michael Johnson, Danling Wang, Anna Schornack, North Dakota State University Department of Civil and Environmental Engineering

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466, Sanford Health, and NASA EPSCoR

Acetone content in exhaled breath of individuals as a biomarker for diabetes has become widely studied as a non-invasive means of quantifying blood-glucose levels. Traditional gas detection systems such as the GC/MS are known to have limitations of size, cost, and response time. Here, we present a novel chemiresistive sensor using a newly synthesized nanocomposite, K2W7O22 nanorods/Ti3C2 nanosheets, to detect exhaled acetone with excellent sensitivity, selectivity, and response time for diagnosing and managing diabetes.

Materials Research

One-pot Synthesis of Ruthenium Nano-catalyst for High-Efficiency Ammonia Production

Wen Sun, Nihat Sahin, Di Sun, Xu Wu, Jivan Thakare, Ted Aulich, Jin Zhang, Xiaodong Hou, Julia Xiaojun Zhao, University of North Dakota Chemistry Department

Sponsor: Department of Energy

Ammonia production consumes significant energy supplies and causes enormous CO2 emissions. In this work, a facile and environmentally friendly one-pot synthetic method for ruthenium-based nanocatalyst has been developed using the reduced graphene oxide as matrix (Ru/rGO). The synthesized Ru/rGO with a Ru-NPs sizes of 2 nm and the metal content of 20 wt.%. The maximum Faradaic Efficiency of 5.3%, the highest ammonia production rate of 0.03 mg/h/mg(cat.) have been reached.

Size-dependent Structural Behaviors of Crumpled Graphene Sheets

Yangchao Liao, Zhaofan Li, Fatima, Wenjie Xia, North Dakota State University Civil and Environmental Engineering Department

Sponsor: ARO, NASA

We present a coarse-grained molecular dynamics study for investigating structural behaviors of graphene sheets having varying sizes during the crumpling process. We found that the structural properties (e.g., the radius of gyration and hydrodynamic radius) can be quantitively described by the power-law scaling relationships during the crumpling process. The overall crumpling behaviors of graphene sheets can be characterized by three regimes, which are associated with edge-bending, self-adhesion, and further compression mechanisms, respectively.

The Atomistic Simulation of Absorbed Water on the Thermomechanical Properties of Crosslinked Epoxy Networks Using Reactive Molecular Dynamics

Anas Karuth, Wenjie Xia, Bakhtiyor Rasulev, North Dakota State University Coatings and Polymeric Materials Department

Sponsor: EPSCoR

The atomistic scale simulation of cross-linking process within polymeric systems is conventionally carried out by connecting reactive sites of monomer. This does not capture the reaction pathway from reactants to final products through transition states. The ReaxFF reactive force field framework that applied in molecular dynamics simulations is used to provide the reactants with a sufficient amount of energy equivalent to or slightly larger than their lowest reaction barrier energy, to overcome the barrier for cross-linking. The reactive molecular dynamics method allows the simulation of the realistic crosslinked polymeric network at a computationally accessible time scale. This framework is implemented to crosslink the diglycidyl ether bisphenol A (BisA) with aliphatic amine (JEFAFMINE D-230) and aromatic amine (DETDA) to achieve a reasonably high crosslink percentage (70%). It is well known that water diffusion through cross-linked epoxy polymers seriously affects the durability of epoxy coatings and accelerates the corrosion of the substrate. In this study, the effect of water absorption on thermo-mechanical properties of epoxy networks was investigated. The interplay between free volume effects and hydrogen bonding interactions is analyzed for the deterioration and recovery of elastic modulus of the epoxy networks. It is observed that water molecules tend to locate within the proximity of polar groups of epoxy networks and have a propensity to aggregate at higher water content. The diffusion coefficient of water in a croslinked epoxy network increases with water content. The ReaxFF framework is also utilized to investigate the hygrothermal

degradation of the crosslinked epoxy network. The JEFAFMINE D-230 cured epoxy network is more susceptible to hydrolytic degradation than DETDA cured epoxy network. This lower hydrolytic degradation of DETDA cured epoxy polymers is accounted for the inaccessibility of water molecules to interact with ether linkages in the DETDA cured epoxy network. The results from performed simulations can help to understand the cross-linked polymers' properties, as well as characteristics of water absorption in epoxy networks, to guide designing new cross-linked epoxy polymers with desired properties to broaden the applications of epoxy materials, including humid environments.

Sustainability considerations in process development and commercialization of Soybean Oil-Based Acrylic Monomers

Na Wu, Zoriana Demchuk, Andriy Voronov, Ghasideh Pourhashem, North Dakota State University and Coatings and Polymeric Materials Department

Sponsor: NSF EPSCoR

(Acryloylamino)ethyl soyate is a soybean oil-based acrylic monomer with versatile properties for polymeric materials applications. In this study, we use TEA and LCA to explore the economic feasibility and environmental performance of the bio-based monomers as a potential replacement for the commercial petro-counterpart. Based on the process model under varying process conditions (different renewable content, catalysts, soybean oil-based feedstocks, and scales), the results highlighted the key technical parameters for improving the sustainability.

Frontal Polymerization of a Thin Film on Wood Substrate

Karan Bansal, Mohiuddin Quadir, John A. Pojman, Dean C. Webster, North Dakota State University Coatings and Polymeric Materials Department

Sponsor: ND EPSCoR, NSF, NIH, NIGMS

Curable coatings with high solid content can address several challenges of coating processes, including generation of VOC and uncontrolled curing. To address these challenges, we formulated coatings which can be cured via frontal polymerization. Frontal Polymerization has been studied extensively as an on-demand polymerization method, which allows one-pot formulation that can support a self-propagating reaction zone. We developed frontally polymerizable resins which can cure on-demand on a wood substrate with application of heat.

Synthesis and Characterization of Steel-MAX Composites

Emily Dahlke, Abdulrahman Aldossary, Caleb Matzke, Daniel Trieff, University of North Dakota Mechanical Engineering Department

Sponsor: UND Army CRADA

Fuel pump components have tribological issues like wearing and scuffing. The objective of this project is to design a high-performance steel composite that is reliable for this application. During this process, we are designing composites of Cr2AlC with 100Cr6 steel by powder metallurgy process. In this poster, we will present the microstructure, mechanical, and tribological behavior of these composites.

Scaffolds Used in Tissue Engineering - An Overview

Erica Eades, Surojit Gupta, University of North Dakota Mechanical Engineering Department

Sponsor: None

To improve healing rates of bone disorders and conditions, researchers suggest engineering bone tissue with scaffolds. Polymeric, ceramic, metallic, and composite materials are all viable options for creating scaffolds. The success of each scaffold can be linked to the material's biocompatibility, mechanical properties, and porosity characteristics. Researchers suggest composite materials hold the most promise, as advantages of each material can be combined. In this poster, we will review some recent advances in scaffold design.

Physics and Astronomy

Probing Electrical Properties of Silicon Nanocrystal Thin Film Using Non-contact Methods; X-ray Photoelectron Spectroscopy and Electrical Circuit Modeling

Amrit Laudari, Sameera Pathiranage, Salim A. Thomas, Reed J. Petersen, Kenneth J. Anderson, Todd A. Pringle, Erik K. Hobbie, Nuri Oncel, University of North Dakota Physics Department

Sponsor: None

We measured XPS while applying DC or AC external biases to a thin film of Si nanoparticles. For conducting samples, the shift in the binding energies of XPS peaks is equal to the external bias. However, for samples with dielectric properties, the shift in the binding energies is smaller than the applied voltages. We used experimental data and an equivalent circuit model to extract the capacitance and resistance of the thin film of Si nanoparticles.

Cr-modified Si (110) Surfaces

Sameera Pathiranage, Rasika N. Mohottige, Nuri Oncel, University of North Dakota Physics Department

Sponsor: EPSCoR

Chromium Silicide is an important refractory metal silicide with high thermal power and a narrow bandgap. The present work investigates the early stages of the growth of Cr film on Si (110) and its electronic properties by combining Scanning Tunneling Microscopy and Density Functional Theory. Scanning Tunneling Spectroscopy measurements showed that the crystallites were metallic. Simulated DOS data of the facets also confirmed the metallic nature of the crystallites.

On the Physics and Chemistry of the Lithiation/Delithiation Process of Cr2S3 and Cr2Se3

Jacob Bogenschuetz, Deniz Cakir, Xiaodong Hou, Michael Mann, Nuri Oncel, University of North Dakota Physics and Department

Sponsor: EPSCoR, UND College of Arts and Sciences

We synthesized Cr2S2 (-Se3) in vacuum-sealed quartz tubes. Both materials have rhombohedral structure with R3 space group. We have investigated the electrochemical performance of these materials as working electrodes. The initial reversible capacity reaches up to 800 mAh/g (700 mAh/g) at the end of the 1st lithiation cycle for Cr2S3 (Cr2Se3) which is significantly better than the graphite-based anodes used in commercial batteries. Moreover, they exhibit better cyclability compared to the other Cr-sulfides.

Chemotherapeutic Drug-induced Dynamics of Cellular Structure in Normoxia and Hypoxia Probed by Atomic Force Spectroscopy

Lina Alhalhooly, Babak Mamnoon, Jiha Kim, Sanku Mallik, Yongki Choi, North Dakota State University Physics Department

Sponsor: NIH/NIGMS (1P20GM109024), ND EPSCoR

Biomechanical properties of several cancer cells after exposure to standard chemotherapeutic drugs were probed by atomic force spectroscopy under normoxic and hypoxic condition. We observed a significant change in cellular stiffness, cell height, surface roughness, and cytoadhesion, demonstrating direct and indirect effects of the drugs on cytoskeletal structure. The overall change in cell stiffness was slower and gradual in hypoxia, suggesting that hypoxia might contribute to drug resistance in context of the tumor microenvironment.

Vacuum Battery Driven Trajectories of Fluid in the Microfluidic Devices

Sung Oh Woo, Myungkeun Oh, Kyle Nietfeld, Bailey Boehler, Yongki Choi, North Dakota State University Physics Department

Sponsor: NIH/NIGMS (1P20GM109024), ND EPSCoR

Integration of the power unit for driving fluid into microfluidic devices is essential for on-chip, droplet blood testing applications. Here, we provide an analytic model to predict fluid driven by vacuum battery, consisting of polydimethylsiloxane (PDMS) membrane and vacuum pocket, in the PDMS microfluidic devices. Furthermore, we provide a prototype of vacuum battery unit that is attachable to devices and controls the trajectory of fluid and show experimental results that fit with the model.

Psychology

Extraversion Differences in Young Adults

Sena Dossou-Gouchola, Michelle Duffy, Dimitry Poltavski, University of North Dakota Psychology Department

Sponsor: Marc U-Star Program

Past research has shown differences in negative affect (depression, stress, and anxiety) between introverts and extroverts. We examined the relationship between extravert status with stress, depression, and anxiety in college students. Our results found a significant difference between introverts (M=7.43) and extroverts (M=3.89), but not ambiverts (M=4.83) in depression levels. Our results showed no differences with stress and anxiety levels between extroverts, introverts, and ambiverts.

STEM Education and Learning Research

Effect of Sleep Quality on Adolescent Appetite, Dietary Intake, and Body Mass Index

Janell Juelich, Dr. Glenda Lindseth, Advisor, University of North Dakota Nursing Department

Sponsor: EPSCoR

Purpose: to examine the effect of sleep quality, quantity, latency, and hygiene on appetite, diet, and BMI. Sample: 76 adolescents completed the study over five nights. Method: Fitbits and Pittsburgh Sleep Quality Index (PSQI) measured sleep. A Visual Analog Scale measured appetite. Block Kids Food Screener measured diet. Adolescent Sleep Hygiene Practice Scale measured sleep hygiene. Results: 88.2% had good sleep quality; 75% had inadequate sleep time; 73.7% had short sleep latency.