ND EPSCoR

FARGODOME
FARGO, NORTH DAKOTA
WEDNESDAY, MARCH 29, 2023

2023 STATE CONFERENCE AGENDA AND ABSTRACT BOOK

NDSU LAND ACKNOWLEDGEMENT

We collectively acknowledge that we gather at NDSU, a land grant institution, on the traditional lands of the Oceti Sakowin (Dakota, Lakota, Nakoda) and Anishinaabe Peoples in addition to many diverse Indigenous Peoples still connected to these lands. We honor with gratitude Mother Earth and the Indigenous Peoples who have walked with her throughout generations. We will continue to learn how to live in unity with Mother Earth and build strong, mutually beneficial, trusting relationships with Indigenous Peoples of our region.

2023 ND EPSCoR Annual Conference

Wednesday, March 29 ♦ Fargodome ♦ Fargo ND

CONFERENCE OPENING

8:30 to 10:00 a.m.

Ballroom

LAND ACKNOWLEDGEMENT

Hollie Mackey, Ph.D., NDSU
PROSPER Lead

WELCOME

Jolynne Tschetter, Ph.D.
Interim Executive Director, ND EPSCoR

GREETINGS

U.S. Senator John Hoeven, Video remarks

U.S. Senator Kevin Cramer, Statement and Represented by Reid Kemp

Congressman Kelly Armstrong, Video remarks and Represented by Mary Christy

Governor Doug Burgum, Statement

NSF UPDATE

John-David Swanson, Ph.D.
Program Director, NSF EPSCoR

GREETINGS

President David Cook, Ph.D., NDSU

BREAK

10:00 to 10:15 a.m.

STORY OF ND-ACES

10:15 to 11:00 a.m. Ballroom

OVERVIEW NEW DISCOVERIES IN THE ADVANCED INTERFACE OF COMPUTATION, ENGINEERING, AND SCIENCE (ND-ACES)

Session Moderator: John Mihelich, Ph.D., UND, VP Research and Economic Development; ND-ACES Co-Principal Investigator

Overview

Kalpana Katti, Ph.D., NDSU
Mark Hoffman, Ph.D., UND
Lisa Montplaisir, Ph.D., NDSU
Hollie Mackey, Ph.D., NDSU

Center for Cellular Biointerfaces in Science and Engineering (CCBSE)

Sanku Mallik, Ph.D., NDSU, Materials Design at Biointerfaces
Archana Dhasarathy, Ph.D., UND, Cellular Systems at Materials Interface
Deniz Cakir, Ph.D., UND, Computation, Machine Learning, and Predictive Modeling

Promoting Sustainable Partnerships in Education and Research (PROSPER)

Ryan Summers, Ph.D., UND, Education and Workforce Development
Danielle Condry, Ph.D., NDSU, Education and Workforce Development
Giancarlo Lopez-Martinez, Ph.D., NDSU, Broadening Participation

POSTER SESSION

11:00 to 11:45 a.m. Lobby

LUNCH AND KEYNOTE SPEAKER

11:45 a.m. to 1:20p.m. Ballroom

PROJECT ACCESSIBILITY: A CONVERSATION ABOUT DEMYSTIFYING SCIENCE

Annalies Corbin, Ph.D.
Founder, President, and CEO, The PAST Foundation

CENTERING TRIBAL COMMUNITY CONCERNS IN RESEARCH ENGAGEMENTS

PANEL DISCUSSION
1:20 to 2:15 p.m. Ballroom

Moderator
Hollie Mackey, Ph.D., NDSU, PROSPER Lead

Panelists
President Donna Brown, Ph.D., Turtle Mountain Community College
Austin Allard, Ph.D., Turtle Mountain Community College
Brent Voels, Ph.D., Cankdeska Cikana Community College
Carissa Brownotter, Graduate Student, NDSU
Lennel Camuy-Velez, Graduate Student, NDSU

BREAK

2:15 to 2:30 p.m.

PROMOTING SUSTAINABLE PARTNERSHIPS IN EDUCATION AND RESEARCH

PANEL DISCUSSION
2:30 to 3:15 p.m. Ballroom

Moderator
Hollie Mackey, Ph.D., NDSU, PROSPER Lead

Panelists
Justin Walden, Ph.D., NDSU, Communications and Dissemination
Ryan Summers, Ph.D., UND, Education and Workforce Development
Giancarlo Lopez-Martinez, Ph.D., NDSU, Broadening Participation

CCBSE RESEARCH HIGHLIGHTS

RESEARCH BRIEFS
3:15 to 4:00 p.m. Ballroom

Establishing Multicellular Patient-Derived Organoids (PDO) Recreating Tumor Microenvironment?

Jiha Kim, Ph.D., NDSU, Cellular Systems at Materials Interface

Quantum Mechanical Treatment of Cancer Cell Adhesion

Mouhmad Elayyan, UND, Cellular Systems at Materials Interface

Progress in Growing 3D Cultures of MDA-MB-231 Cells

Colin Combs, Ph.D., UND, Cellular Systems at Materials Interface

Investigating the Mechanics and Conformational Changes of Integrins at the Molecular Scale

Hanmant Gaikwad, NDSU, Computation, Machine Learning, and Predictive Modeling

CLOSING REMARKS

4:00 to 4:30 p.m. Ballroom

Colleen Fitzgerald, Ph.D., NDSU, Vice President for Research and Creative Activity;
ND-ACES Principal Investigator and Project Director

Abstract Booklet

Table of Contents

Photography and Videography

Please contact ndepscor@ndu.edu with questions. Photographs will be taken at this event, which may be used on our websites, in our printed materials, and or for other reporting or promotional purposes. If you do not wish to have your photograph taken and used by ND EPSCoR, please alert the photographer.

Acknowledgement

Research presented at this conference was supported by the State of North Dakota and the National Science Foundation under NSF EPSCoR Track-1 Cooperative Agreement OIA #1946202. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

Undergraduate Students

#1 3-D Realistic Reconstruction of Human Breast Cancer Cell Using Patient-specific Data

Ryan Thoreson, Colter Huseby, Lahcen Akerkouch, Trung Le, Amanda Haage, and Aaron Vanyo

North Dakota State University, Department of Civil, Construction and Environmental Engineering; and University of North Dakota Department of Biomedical Sciences

Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

Understanding how breast cells are transported through the body could be help with cancer diagnosis and treatment procedures. While computational studies of cancer metastasis have provided valuable insights into the cancer migration, most previous studies assumed idealized spherical shapes of the cancer cells. Our research objective is to investigate how three-dimensional shape of cancer cells affects their migratory paths using confocal microscopic images.

#2 Cancer prediction using cell-free DNA

Aerica Nagornyuk, Sakuntha D. Gunarathna, Regina Nguyen, Mika Saotome, and Motoki Takaku

University of North Dakota, Department of Biomedical Sciences,

Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

Cell-free DNA (cfDNA) are non-encapsulated DNA circulating in the blood. In cancer patients, some cfDNA populations are known to be released from cancer cells. Research shows that cfDNAs with partially retained epigenetic information can predict cell-of-origin, and by extension, cancerous tissues. Therefore, cfDNA analysis is a promising biomarker for translational studies and noninvasive cancer patient screening. We isolated cfDNA from Sanford Biobank plasma samples and compared breast cancer patient donors and healthy patient donors.

#3 Characterization of Lignin Treated via Oxidation and pH Variation, and Product Effects on Soil Water Retention Capability

Shadlynn Severance and Audrey LaVallie

Nueta Hidatsa Sahnish College

Sponsor(s): NSF ND EPSCoR seed grant

Lignin (a waste product of papermaking) has been considered as a possible soil amendment, in terms of water retention properties. Lignin here was subjected to peroxide oxidation at various pH regimes, in order to produce carboxylic acid groups, alcohols, quinones and carbonyl groups attractive to water. Lignin potential as a water-retention agent was monitored under drought conditions in laboratory plants (ryegrass and wheatgrass) over prolonged periods; several treated lignins showed increases in soil water retention.

#4 Creation of a hyperplane device for horizontal cellular migration assays

Nicholas M. Bittner, Nelofar Nargis, Colin K. Combs, and Brent J. Voels

University of North Dakota, Health Science Department of Biomedical Sciences and Cankdeska Cikana Community College

Sponsor(s): NSF Research Experiences for Undergraduates Site grant 1852459, National Institute of General Medical Sciences NIH grant 8 P20 GM103442-12, NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202, NIH grant P20GM113123, NIH DaCCoTA Center NIGMS U54 GM128729, and UNDSMHS funds

Cell culture studies routinely seek to monitor cell migration in response to chemoattractant stimuli. Common assays of cell migration employ well inserts and vertical cell migration assessment. This approach does not allow real-time monitoring of cell behavior. To address this need, we sought to develop a horizontal culture platform conducive to time course cell assessment changes in migration, morphology, phenotype etc. Modification of a commercial chamber slide allowed us to quantify cell migration in response to a 20% serum gradient. Based upon this finding, we designed and fabricated a prototype chamber slide for high replicate, real time assessment of cell migration in the serum gradient. The novel chamber slide design was effective for quantifying not only cell migration differences but visualizing cell movement. Optimization of the fabricated design will provide a novel tool for cell biology research.

#5 Plant Polymer Arabinoxylan Based Soft Scaffolds for Breast Cancer Cell Growth and Proliferation

Kaydee Koistinen, Md Sultan Mahmud, Michael Kjelland, Abulquasem R. Hossain, Brooke Roeges, Haley Boechler, Julia Kohl, Trevor Gravseth, Alize Pratt, Caden Bjornstad, Sanku Mallik, and Khwaja Hossain

Mayville State University and North Dakota State University

Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

Biopolymers are functional material and among biopolymers arabinoxylans (AX) are the main non-starch polysaccharide in cereals and other plants. AX is composed of xylose, arabinose, and ester linked ferulic acid with arabinose confer it's the bioactive properties. The backbone of AX is like glycosaminoglycans, a major extra cellular matrix of human body. The objective was to identify plant derived AX that is suitable for supporting the growth and proliferation of cancer cell MB231.

#6 Proof of Concept for High-Efficiency and High-Throughput Site-Specific Integration of Synthetic Reporter Genes into the Mouse Genome

Brayden Groll, Manu Manu, Sunil Nooti, and Madison Naylor

University of North Dakota, Department of Biology

Sponsor(s): NSF grant-1942471

Reporter assays are an important tool for studying transcriptional regulation. We established a system for reproducible and quantitative reporter assays using CRISPR/Cas9 to integrate reporter genes in a site-specific and biallelic manner. Here, we report progress in improving the system by creating a landing pad, expressing a fluorescent protein, that is exchanged with the reporter using high-efficiency recombinase-mediated cassette exchange. This strategy should have higher efficiency and throughput since clones can be isolated with FACS.

#7 Rapid Synthesis of N-ethyl-N-[1-(2-naphthyl)ethyl]formamide

Christopher M. Scott, Lioudmila I. Bobyleva, and Mikhail M. Bobylev;

Minot State University, Division of Science – Chemistry

Sponsor(s): National Institute of General Medical Sciences NIH grant 8 P20 GM103442-12 and NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

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-ethyl-N-[1-(2-naphthyl)ethyl]formamide. The reaction was conducted on a 10 mmol scale at 180 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-ethyl-N-[1-(2-naphthyl)ethyl]formamide was 87%.

#8 Rapid Synthesis of N-[1-(2,4-difluorophenyl)ethyl]-N-methylformamide

Monica J. Anderson, Lioudmila I. Bobyleva, and Mikhail M. Bobylev;

Minot State University, Division of Science – Chemistry

Sponsor(s): National Institute of General Medical Sciences NIH grant 8 P20 GM103442-12 and NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

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-(2,4-difluorophenyl)ethyl]-N-methylformamide. The reaction was conducted on a 10 mmol scale at 180-184 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 120 minutes. The isolated yield of N-[1-(2,4-difluorophenyl)ethyl]-N-methylformamide was 80%.

#9 Rapid Synthesis of N-ethyl-N-[1-(4-trifluoromethylphenyl)ethyl]formamide

Lynn I. Vick, Lioudmila I. Bobyleva, and Mikhail M. Bobylev

Minot State University, Division of Science – Chemistry

Sponsor(s): National Institute of General Medical Sciences NIH grant 8 P20 GM103442-12 and NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

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-ethyl-N-[1-(4-trifluoromethylphenyl)ethyl]formamide. The reaction was conducted on a 5 mmol scale at 180-210 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 60 minutes. The isolated yield of N-ethyl-N-[1-(4-trifluoromethylphenyl)ethyl]formamide was 86%.

#10 Rapid Synthesis of N-methyl-N-[1-(4-trifluoromethylphenyl)ethyl]formamide

Branden Z. Pelzer, Lioudmila I. Bobyleva, and *Mikhail M. Bobylev*

Minot State University, Division of Science – Chemistry

Sponsor(s): National Institute of General Medical Sciences NIH grant 8 P20 GM103442-12 and NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

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-methyl-N-[1-(4-trifluoromethylphenyl)ethyl]formamide. The reaction was conducted on a 10 mmol scale at 190-200 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-(4-trifluoromethylphenyl)ethyl]formamide was 93%.

#11 Strontium Isotope Analysis of Great Plains Holocene Bison

Ethan Simons and Igor V. Ovchinnikov

University of North Dakota, Department of Biology

Sponsor(s): ND EPSCoR STEM Undergraduate Research and University of North Dakota Research and Creative Activity Awards, 2022 and 2023

Chemical element isotopes are found in bone and dental tissue. These isotopes can be analyzed, providing insight into the migratory patterns, diets, and environments of an animal. In this study, dental enamel was extracted from Middle and Late Holocene bison molars and the $^{87}Sr/^{86}Sr$ isotopic ratios associated with each tooth were analyzed. Results show statistically significant changes in strontium isotope ratios for Holocene molars in comparison to modern controls, suggesting migratory movement during enamel hardening. Continued research will collect additional samples from archaeological sites across the Northern Great Plains alongside additional modern controls. Cross-referencing of results with other elemental isotopes taken from the same molars will produce accurate life histories of Holocene bison.

#12 Synthesis of N-[1-(6-methoxy-2-naphthyl)ethyl]-N-methylformamide

Daniela Nardelli, Lioudmila I. Bobyleva, and Mikhail M. Bobylev

Minot State University, Division of Science – Chemistry

Sponsor(s): National Institute of General Medical Sciences NIH grant 8 P20 GM103442-12 and NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

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-(6-methoxy-2-naphthyl)ethyl]-N-methylformamide. The reaction was conducted on a 10 mmol scale at 180-186 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 120 minutes. The isolated yield of N-[1-(6-methoxy-2-naphthyl)ethyl]-N-methylformamide was 96%.

Technical Support Staff

#13 Machine Learning, Computational Chemistry and Chemical Substructure Extraction Methods to Predict Photoluminescence Properties of Single-Walled Carbon Nanotubes.

Gerardo M. Casanola-Martin, Amirreza Daghighi, August Amb, Grace Tiffany, Dmitri Kilin, Svetlana Kilina, Bakhtiyor Rasulev

North Dakota State University, Department of Coatings and Polymeric Materials and Department of Chemistry and Biochemistry

Single-walled carbon nanotubes (SWCNTs) are nanomaterials widely used in industrial and biomedical applications. Computational studies are widely applied last coupe decades to investigate physical, chemical, and mechanical properties of carbon nanotubes. Here we report for the first time a data-driven nano-QSAR study for a series of 85 SWCNTs with sp^3 -hybridized defects, in order to investigate and predict photoluminiscence properties SWCNTs. Two Quantitative Structure-Property Relationships (QSPR) models for photoluminescence wavelength (nm) and oscillator strength were generated, molecular structures were used as input information, where encoded information was convalent functional groups and the two base rings. The obtained Multi-Linear Regression models showed performances in the training set (R^2 = 0.978), validation set (R^2 = 0.964) for the Wavelength (nm) and in the case of the Oscillator Strength, the determination coefficients were R^2 = 0.924 and R^2 = 0.872 for training and test set, respectively. The QSPR models were also internally validated by 10-fold cross-validation and Y-scrambling experiments, showing that the models have high levels of goodness-of-fit, robustness and predictivity. The proposed approach provides an important tool to predict the photoluminescence properties of single-walled carbon nanotubes, taking into account only a small portion of the molecular structure avoiding lengthy and complex calculations, for the design/virtual screening of SWCNTs with improved photoluminescence properties.

#14 Effects of 2D versus 3D Culturing on Cellular Morphology and Gene Expression

Jenna Grindeland, Kaitlyn Gura, Carson Herbert, Jarret Merschman, Shrinwanti Ghosh, Giha Kim, Motoki Takaku, and Archana Dhasarathy

University of North Dakota, Department of Biomedical Sciences

Sponsor(s): DaCCoTA to AD and MT, ND-EPSCOR URA program to CH, NIH DaCCoTA Center NIGMS U54 GM128729 and 2P20GM104360-08A1, and NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

Relative to 2D cell culture, growing breast cancer cells in 3D culture systems have been found to more closely mimic *in vivo* tumor environments. The goals of our project are to assess the efficiency of two different methods of 3D culturing for cancerous and non-cancerous cell types, as well as comparing 2D versus 3D differences in cellular morphology. We will use 3D culture systems to study gene expression and the epithelial-mesenchymal transition (EMT), a key process involved in cancer metastasis and drug resistance.

#15 Rapid Synthesis of N-[1-(4-trifluoromethylphenyl)ethyl] formamide

Hassan S. Elshanbary, Lioudmila I. Bobyleva, and Mikhail M. Bobylev

Minot State University, Division of Science – Chemistry

Sponsor(s): National Institute of General Medical Sciences NIH grant 8 P20 GM103442-12 and NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

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-trifluoromethylphenyl)ethyl] formamide. The reaction was conducted on a 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-[1-(4-trifluoromethylphenyl)ethyl] formamide e was 76%.

Graduate Students

#16 3D in-vitro Cancer Model Picturing Cellular Crosstalk and Bone Metastasis

Shrinwanti Ghosh, Sangdeuk Ha, Jiha Kim, Kalpana Katti, and Anu Gaba

North Dakota State University, Department of Biological Sciences and Department of Civil Engineering; Sanford Roger Maris Cancer Center

Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

Cancer cells proliferate, adopt to environment, and spread to adjacent or distant organs. Multi-cellular communication during this process critically impacts tumor progression and metastasis. Aim of this study was to create *in vitro* tumor microenvironment through multicellular co-culture system to investigate influence of vascular components on cancer cell dynamics. 3D spheroid of patient-derived breast cancer cells were co-cultured with endothelial cells and pericytes. Morphological and molecular changes of all cell types were investigated. Long-term objective of this study is to develop 3D scaffold culture systems to investigate development of bone metastatic tumors.

#17 A Fast Charging Technique for Lithium Ion Battery at Freezing Temperature

Shabaz Khan, Xiaodong Hou, Daniel Laudal, and Michael Mann

University of North Dakota, Institute for Energy Studies, College of Engineering and Mines

Sponsor(s): ND EPSCoR seed funding and NSF I-Corp

The two most significant obstacles to Electric Vehicle (EV) growth are range anxiety and recharging time. Our proposed fast-charging method is operational at freezing temperatures. The goals are: 1) charge a battery to 90% within 15 minutes, and 2) keep battery cycle life longer. Our fast-charging technique can charge the battery at freezing and room temperature. The wide range of applications made it easy to apply for different temperatures.

#18 A Joint Modeling Framework for Simulating Hydrologic Processes in a Wetland-influenced Watershed

Tiansong Qi, Mosammat Mustari Khanaum, Kyle D. Boutin, Marinus L. Otte, Xuefeng Chu

North Dakota State University Department of Civil, Construction and Environmental Engineering and Department of Biological Sciences

Sponsor(s): United States Environmental Protection Agency (USEPA)

It is a challenge to incorporate the influences of individual small wetlands into a watershed-scale hydrologic model by using a lumped method for wetland parameterization. To overcome the challenge, a joint modeling framework was proposed to couple a surface delineation algorithm with a semi-distributed hydrologic model. It was then applied to a wetland-influenced watershed in North Dakota. The results demonstrated its capability and improvement in the modeling of hydrologic processes under the influence of wetlands.

#19 A Multi-objective Model Formulation for Corn Supply Network: A Case Study Based on North Dakota

Labiba Noshin Asha, Nita Yodo, and Harun Pirim

North Dakota State University, Department of Industrial and Manufacturing Engineering

Sponsor(s): ND EPSCoR, North Dakota Corn Council, North Dakota Soybean Council, and North Dakota State University

A multi-objective model is developed to reduce total cost and CO2 emissions in the supply network between corn production zones and ethanol plants in North Dakota, using real-time data to validate it. The ε-constraint method was used to simplify the model, showing that harvesting techniques utilized in different production zones impacted the costs and emissions. This highlights the need to consider both factors in decision making activities for sustainable corn production and supply chain management.

#20 A QSPR approach to mask the bitterness of wheat bran and wheat bran products via incorporating phenolic acids into beta-cyclodextrin to form bio-complexes.

Kweeni Iduoku

The need for solvating and encapsulating hydro-sensitive molecules drives the trend of applying cyclodextrins to food, pharmaceuticals, polymers, materials, and the agricultural sciences. In food and agricultural science, alpha, beta, and gamma cyclodextrins are used the most. In a previous study, our predecessors used the entrapping properties of beta-cyclodextrins (BCD) to mask the bitterness of wheat bran. Hence, this research focuses on reducing the bitter perception of wheat bran during consumption by employing machine learning methodologies like cheminformatics alongside statistical tools. It addresses the encapsulation mechanism of the BCD-ligand complex and develops a model that dictates the descriptors with the most influence on the BCD-ligand complex. Additionally, this study investigates the predictive capacity of our models by predicting the properties of new ligands that are structurally and chemically related to the dataset used. For these benefits, our study strives to go beyond the boundaries of wet chemistry with computational and statistical methodologies.

#21 Ab initio investigation of bio-interfaces between iron and magnesium doped nano-montmorillonite clay and unnatural amino acids

Warnakulasuriya Ashan Fernando, Mark Hoffman, and Deniz Cakir

University of North Dakota, Department of Physics and Astrophysics and Department of Chemistry

Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

We performed a density functional theory study of 11 different unnatural amino acids to understand their interaction with Fe and Mg co-doped montmorillonite nanoclay. We identified the amino acids interacting strongly with the clay surface by calculating binding energies, and they indicate a substantial electrostatic interaction between the acid molecules and the clay slab, with the amino group being dominant. Also, the inclusion of a solvent was shown to enhance the binding energy of amino acids on the clay slab.

#22 Adsorption and reactions of SO_2, H_2S, C_4H_4S, and CO on Graphene and Pt/Graphene

Thomas Stach and Uwe Burghaus

North Dakota State University, Department of Chemistry and Biochemistry

Sponsor(s): 2022 ND NASA EPSCoR Supplemental Project Funding Award

The adsorption of H_2S, SO_2, and C_4H_4S at ultra-high vacuum conditions were studied on graphene epitaxially grown on Ru(0001) using thermal desorption spectroscopy (TDS) and Auger electron spectroscopy (AES). Multi-mass TDS data deviates from the gas phase fragmentation pattern, suggesting that the molecules undergo a chemical transformation. AES revealed adsorbed sulfur on the surface after the TDS experiments for all probe molecules. Adsorption experiments of CO on platinum clusters grown on graphene/ruthenium are underway.

#23 Analysis of Ground and Excited State Pair Spatial Localization Towards Understanding the Photodegradation in Polymers

Meade Erickson, Yulun Han, Gerado M. Casañola-Martin, Bakhtiyor Rasulev, and Dmitri Kilin

North Dakota State University Department of Coatings and Polymeric Materials and Department of Chemistry and Biochemistry

Sponsor(s): NSF ND EPSCoR Track-1 grant II-A-1355466, and NSF grant CHE-1944921

Photodegradation of polymers is a complex phenomenon that is influenced by both topological and electronic structure of polymers. Regarding the process of exciting an electron from ground to excited state for photodegradation to occur, it is known that various relationships are expected to exist between ground and excited states. The goal of this work is to establish quantitative relations between density functional theory calculated rate of photodegradation, defined as inverse duration of irradiation by light of certain wavelength and intensity, and several factors describing polymer geometry and electronic structure. Specific factors, including oscillator strength and transition energy of excitations matching resonance condition with incident radiation, have already been shown to influence the rate of photodegradation. Another factor that is believed to affect the rate of photodegradation is the spatial localization between the two orbitals relative to each other and along the structure. To investigate the influence of spatial localization on rate of photodegradation, we employ a cooperative approach between time dependent excited state molecular dynamics (TDESMD) and cheminformatics techniques where topological information is used to help describe the influential path of electron movements.

#24 Analyzing the Impact of Pre-training Datasets and Fine-tuning on Cancer Histopathology Images using Transfer Learning

Koushik Howlader and Lu Liu

North Dakota State University, Department of Computer Science

Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement-OIA-1946202

Transfer learning is often utilized in medical imaging models due to the lack of training data. This study examines the impact of transfer learning on cancer histopathology imaging by evaluating three deep neural networks on three target datasets. The study concludes that pre-training with ImageNet or random initialization is more effective than pre-training with cancer histopathology image datasets. Additionally, the study finds that increasing the number of images used in fine-tuning can improve the performance.

#25 *Azospirillum brasilense* Sp7 swimming motility towards specific root exudate compounds

Fatema Akter Nisha, Shelley M. Horne, and Birgit M. Pruess

North Dakota State University, Department of Microbiological Sciences

Sponsor(s): USDA/NIFA Specialty Crop Block Grant

The free-living, nitrogen fixing *Azospirillum* is one rhizobacteria that aid in plant's growth by travelling toward the plant's roots exudates and colonizing the roots. The swim plate assay was used to examine the chemotaxis of *Azospirillum brasilense* to known compounds of plant root exudates that might serve as chemoattractants for the bacteria. The production of concentric rings indicates chemotaxis towards the compound. The best performance of *A. brasilense* Sp7 was observed with fructose and succinate.

#26 Biodegradable Conjugated Polymer Nanoparticles (Pdots) for Biological Imaging

Chiranthi Mahadurage, Julia Zhao, and Guodong Du

University of North Dakota, Department of Chemistry

Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

Bioimaging is a powerful technique for understanding biological processes and malfunctions. Conjugated polymer nanoparticles (Pdots) for fluorescence imaging are highly sought after in due to their excellent light-harvesting performance, high biocompatibility, and tunable molecular structure. However, the main concern related to most Pdots is lack of biodegradability. Our focus is to design and synthesize novel biodegradable Pdots for biological imaging.

#27 Bone Mimic Scaffolds As a Model for Understanding *In Vitro* Microenvironments of Metastatic Cancer Niche

Matthew Johnston, Amanda Haage, and Aaron Vanyo

University of North Dakota School of Medicine and Health Sciences

Biomaterials such as bone scaffolds and polyacrylamide hydrogels serve to mimic in-vivo microenvironment for more accurate analysis of metastatic behavior. A nano-hydroxyapatite-clay (HAP MMT-Clay) scaffold with a novel production method was developed as an in vivo bone mimic environment. This scaffold was found to be a viable material for the culture, proliferation, and differentiation of cells. Bone is a common site of cancer metastasis and therefore utilizing biomaterials that mimic bone to further study metastatic transition of cancer cells is valuable. Mechanisms for bone metastasis include epithelial to mesenchymal transition, micro-environmental support, and vascular adhesion and extravasation. Furthermore, a polyacrylamide hydrogel procedure was initiated in house with goals of creating tunable cell culture substrates to mimic different organoid stiffness.

#28 Cardiac Specific PPARα knock-out Protects Against Cardiac Lipid Accumulation During Metabolic Stress

Savannah Gibson, Kaleb Barnes, and Natasha Fillmore

North Dakota State University, Department of Pharmaceutical Sciences

Sponsor(s): ND EPSCoR

Obesity contributes to cardiovascular disease; however, the mechanism remains elusive. PPARα has been linked to cardiovascular diseases. Here we used our novel cardiac specific PPAR KO (cPPAR$^{-/-}$) mouse. Mice were either fasted or fed 5wk HFD. HFD fed cPPAR$^{-/-}$ vs Ctrl hearts have lower TG and Plin2. We also found a compensatory increase in Plin3 and DGAT1 in cPPAR$^{-/-}$ hearts. These results indicate that cPPAR$^{-/-}$ protects the heart from fat accumulation and regulates perilipins.

#29 Comparative study of photoluminescence of single and ensemble oligomers of cis-polyacetylene semiconductor materials

Kamrun N. Keya, Wenjie Xia, and Dmitri Kilin

North Dakota State University, Department of Chemistry and Biochemistry, and Department of Civil, Construction and Environmental Engineering

Sponsor(s): National Energy Research Scientific Computing Center, NSF ND EPSCoR, NSF CHE-1944921, and Department of Energy DE-SC0021287

Semiconducting conjugated polymers (CPs) have shown great potential in organic solar cells and organic field-effect transistors (OFETs) due to their tunable electronic and optical properties. Photoluminescence (PL) is one of the key observables in experimental characterizations of optoelectronic materials, including CPs. In this study, two different models of cis-polyacetylene (single cis-PA oligomer and ensemble of cis-PA) are used to explain the mechanism of PL of the CPs. The photo-induced excited state dynamics are computed using a combination of the ab initio electronic structure and time-dependent density matrix methodology[1]. We explore the phonon-induced relaxation of the excited states. Here, the dissipative Redfield equation is used with the nonadiabatic couplings as parameters. The simulated results for both models show that the relaxation rate of the electron is found to be faster than the relaxation rate of the hole. The dissipative excited-state dynamics are combined with radiative recombination channels to predict the PL spectrum. The simulation results reveal similarities and differences in the absorption and emission spectra for single and multiple oligomers[2].The main result of the single oligomer is that the computed PL spectrum demonstrates two mechanisms of light emission originating from (i) the inter-band transitions, corresponding to the same range of transition energies as the absorption spectrum, and (ii) intra-band transitions which are not available in the absorption spectra[2,3]. This work compares the spectroscopic signatures of a single cis-PA oligomer versus an ensemble of such oligomers. Formation of the ensemble results in noticeable changes in transition energies and intensities of transitions for both absorption and emission spectra. As the excited state charge density changes over time, ensembles of cis-PA demonstrate processes of charge density localization and delocalization. These results can be used for improving organic semiconductor materials for photovoltaic and LED (light emission diode) applications.

#30 Comparison of Quantum Chemical Methods for Some Biological Molecules

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Sponsor(s): NSF EPSCoR grant OIA-1355466

Density functional theory (DFT) has become one of the most popular quantum chemical models in the last few years. For the investigation of the electronic structure of ground state molecules, DFT offers a less expensive alternative than wavefunction-based methods that include correlation effects (e.g. MPn). The accuracy of gradient-corrected DFT functionals is often about the same as that of MP2. However, in some cases of reactions involving H-atoms, DFT fails to predict reaction barriers. Considering these facts, one should handle DFT as a method that should be applied by paying special attention to the problem under investigation, keeping in mind the model's limits. In this work, we investigated the difference between DFT (PBE & B3LYP) and MPn using 10 different amino acids. Our investigation showed that DFT methods which are less expensive gave similar results to those of MPn except for one molecule where its dipole moment and geometric parameters were different from those of MPn. Thus, further study is needed to characterize the onset of differences between DFT and MPn in biological or biomimetic systems.

#31 Computational Methods for Predicting the Water Permeability of Bio-based Polymer Thermoplastics

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North Dakota State University Department of Coatings and Polymeric Materials

While plastic pollution poses a significant ecological threat, replacing petroleum-based plastics with bio-based ones can improve sustainability. However, their water permeability characteristics require further study for utilization in various applications, including food packaging and medicine. Since experimental assessment of water permeability properties are time-consuming, computational approaches can be very helpful to at least reduce number of experiments. We present here computational methods as an integrated approach, combining molecular dynamics simulations and machine learning, to gain insight into the permeation behavior of bio-based polymer thermoplastics, promoting a more sustainable and eco-friendly approach to plastic production.

#32 Dual Functional Near-infrared Fluorescent Polymer Dots-siRNA Nanomedicine for Cancer Gene Therapy

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Sponsor(s): NSF grant CHE 1709160; NSF ND Cooperative Agreement Award OIA-1946202; NIH COBRE grant Pilot Project (2P20GM104360-06A1; P.I. R. Vaughan); Multi-Investigator Seed Grant from the College of Arts and Sciences (JXZ and DCD) AND Pilot Project Grant P20 GM104360 Epigenetics of Disease and Development (JXZ and DCD)

RNA interference (RNAi) mediated by siRNA is a promising gene therapy strategy for cancer or other genetic disease treatment. To date, the clinical trial is still facing several challenges, including metabolic instability, low delivery efficiency, poor cellular uptake. To address these challenges, we have explored a dual functional polymer dots (Pdots) nanoplatform for both practical deliveries of GAPDH-siRNA and in vitro monitoring of delivery via strong NIR fluorescence from Pdots nanoplatform.

#33 Effects of Corn Oil Derived Surfactants on Corrosion Rate

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Sponsor(s): North Dakota Corn Council

This study investigates the synthesizing of corn oil-based surfactants and further investigates their influence on the surface properties. Four types of bio-surfactants were synthesized through different reactions using potassium hydroxide and sodium hydroxide. The produced bio-surfactants were characterized using (FT-IR) and (NMR). The influence of concentration on corrosion inhibition in brine solution was tested. The FT-IR and NMR analysis confirmed the proposed structure. The results showed that the products efficiently reduced the corrosion rate.

#34 Efficient Last-Mile Delivery System for Emergency Supplies Using Trucks and Drones: A Cooperative Routing Approach

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North Dakota State University, Department of Industrial and Manufacturing Engineering

Sponsor(s): ND EPSCoR and North Dakota Corn Council

In the aftermath of a disaster, affected people need timely delivery of emergency supplies to minimize potential casualties. A last-mile distribution system is modeled for delivering emergency supplies as a cooperative two-echelon routing problem, where trucks and drones work together to optimize the delivery routes. A novel greedy randomized adaptive search procedure with a path relinking framework is proposed to solve the problem promptly. The effectiveness of the proposed framework is demonstrated through experimental results. The proposed system not only minimizes the delivery time but also optimizes the utilization of resources, making it a viable solution for emergency response efforts.

#35 Efficient Monte Carlo Simulation of Fluorescence Microscopy in Neural Tissue

Cecilia Ling and Bo Liang

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Sponsor(s): ND EPSCoR ND-ACES Cyberinfrastructure (CI) Assistantship Award through NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

The application of machine learning techniques in microscopic image restoration achieved superior performance. However, the demand for large dataset and lack of ground truth hindered its development. Our study utilized computer simulation model the neural anatomic volume, fluorescence light transportation inside tissue volume and photon collection process of microscopic imaging sensor aimed at generating realistic image data for the training and validation of machine learning model. The images produced by the simulator showed promising results.

#36 Electrospray Ionization High Resolution Time-of-Flight Mass Spectrometry: an Effective Analytical Technique to Characterize Synthetic Polymers

Md Redwanul Islam, Anastasia Andrianova, and Md Musfiqur Rhaman Alena Kubatova

The idea of ESI-HR-TOF-MS is ionizing the analyte molecules with electrospray followed by the measurement of mass-to-charge ratio with time-of-flight mass spectrometer. ESI-HR-TOF-MS provides accurate MW ranging from small to high MW. However, this technique was not extensively explored to characterize synthetic polymers. In this work, we explain a unique method to determine MW as well as charge of polymer ions which can be very useful for characterization.

#37 Exploring the Thermomechanical and Interfacial Behaviors of Clay-Arabinoxylan Nanocomposite: A Molecular Dynamics Study

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Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

Clay minerals have attracted widespread attention due to their different applications in industry such as drug-delivery system, catalyst supports, templates in organic synthesis, cosmetics, wastewater treatment, and petroleum industry. The fundamental understanding of biomolecule-clay interaction is of great relevance to the drug-delivery and cancer biology industries. To this end, we employed molecular dynamics (MD) to capture the molecular features of arabinoxylan (AX) and the most common type of clay mineral, sodium-montmorillonite (Na-MMT) in the presence of water molecules (Figure 1). We utilized all-atomistic (AA) models in this work because they are more accurate and better depict the interaction between particles by taking into account interatomic coulombic interactions. The outcomes of this work address challenges for the advancement of numerous cutting-edge MMT mineral applications in the fields of cancer biology and biotechnology. For example, tissue engineering involves the expansion of cells from a small biopsy, followed by *in vitro* cell culturing in temporary three-dimensional (3D) scaffolds. For this study, human breast cancer cells (MDA-MB-231, ATCC®) were procured for cell culture.

#38 Finite element analysis of biomarker separation using deterministic lateral displacement

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North Dakota State University, Department of Physics

Sponsor(s): NIH/NIGMS 1P20GM109024

Efficient separation of target biomarkers from biofluids such as whole blood is essential for the development of molecular diagnostic devices. Particle separation techniques based on the deterministic lateral displacement (DLD) principle have shown promise in overcoming poor quality and low yield issues associated with conventional ultra-centrifugation and size-exclusion methods. Using finite element analysis, we investigate the principles of particle separation and trajectory in DLD-based microfluidic devices and demonstrate the feasibility of its practical applications.

#39 First principle investigations on the surface interaction of amino acids with Fe-Mg co-doped montmorillonite (MMT) nano-clay

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North Dakota State University, Department of Chemistry and Biochemistry

Sponsor(s): NSF ND EPSCoR Track-1 OIA-1946202

Amino acids are the building block of proteins and have been widely used as the prototype to model various types of proteins. In this work, the interaction of amino acids with Fe-Mg doped montmorillonite (MMT) clay molecule, in vacuum as well as in aqueous medium, have been extensively studied in terms of conformational distribution, binding affinity and magnetic properties. The aqueous medium enhances the adsorption of amino acid forming a complex network of H-bonding with surrounding water molecules. The role and impact of the adsorption of the amino acids on the clay minerals is of great importance to understand its implications on electromagnetic and biomedical applications. Using the first principal density functional theory, we are interested to study the interaction of amino acids at the surfaces of the Fe-Mg doped MMT clay mineral (CM) with empirical chemical formula $(FeMg)_{0.25}Al_{1.5}Si_4O_{10}(OH)_2.nH_2O$ in which Fe and Mg both exist in +2 oxidation state. The proposed amino acids (AA) for the adsorption are a) 5-Aminopentanoic acid (5-Aminovaleric acid), b) 2-Aminoheptandioic acid (2-Aminopimelic acid), and c) (2-Aminooctanoic acid (D L-2-Aminocaprylic acid). The figure alongside represents the pristine (a) bulk and (b) slab structures of MMT clay, Where T and O represents tetrahedral and octahedral sheets respectively. It is hoped that alternative amino acid substitutes with existing medical uses will allow for correction of charge density issues arising from unequal charge distribution.

#40 Ground and Excited State Properties of Charged Non-Stoichiometric Quantum Dots

Omolola Eniodunmo, Svetlana Kilina, Sergei Ivanov, Dibya Ghosh, and Sergei Tretiak

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Sponsor(s): Los Alamos National Laboratory Project 20200213DR, Indian Institute of Technology Delhi SEED Grant PLN12/04MS, NSF grant 2004197, and ND EPSCoR

Colloidal Semiconductor Quantum dots are nanocrystalline structures that are used for several applications due to their highly size-tunable properties. We use density functional theory (DFT) and time-dependent DFT(TD-DFT) with hybrid functional B3LYP to explore different methods (dangling bond and doping) of creating charged non-stoichiometric cadmium selenide (CdSe) clusters and their effect on the ground and excited state properties. Results show that ligand removal is similar to electron doping for Cd-rich but hole doping for Se-rich.

#41 Harnessing Interpretable Machine Learning to Predict Cancer with Cell-Free DNA

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Sponsor(s): DaCCoTA Pilot Projects, NIH COBRE P20, and NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

In cancer patients, certain populations of cell-free DNA (cfDNA) are known to be released from cancer cells and retain genetic and epigenetic information of the cell origin. Several machine learning algorithms are currently being developed to better understand how this epigenetic data might be used to predict cancer patient outcomes. Using cfDNA data from breast cancer and healthy donors, we developed an interpretable computer model and achieved a high prediction accuracy (Validation: 94%; AUC: 92%).

#42 How is green and sustainable chemistry integrated into the undergraduate organic chemistry curriculum across the United States?

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Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202 and NSF Division of Undergraduate Education 2021285

Despite the growing emphasis on integrating green and sustainable chemistry (GSC) into the curriculum, it is not well-represented in organic textbooks. Thus, the decision of what aspects and how to incorporate GSC is left to the instructors. To discover what aspects of green chemistry, planetary boundaries, and the UN SDGs are currently integrated and what factors affect its integration, we surveyed organic faculty from across the United States. This poster will address the study findings.

#43 Insights into Actin Filament Severing Mechanism by ADF/Cofilin: A Molecular and Structural Study

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Sponsor(s): NSF grants 1229316 and 2019077, and NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

The cytoskeleton maintains eukaryotic cell shape and mechanical rigidity. In cancer, cytoskeletal changes affect cell deformation mechanics and motility. Dynamic actin cytoskeleton reorganization is required for metastatic cancer cell spread. In this study actin filament mechanics were investigated using steered molecular dynamics simulation, revealing that deformation response is regulated by dissociation of conformational locks at intra-strand and inter-strand G-actin interfaces. ADF/Cofilin alters actin structure, changing physical properties. These findings are important for constructing a mechanobiological cell model to mimic disease progression.

#44 Integrative Analysis of Epigenomic, Transcription Factor, and Hi-C Data to Identify Genomic Differences in Prostate Cancer Cell Lines

Chanaka Bulathsinghalage and Lu Liu

North Dakota State University, Department of Computer Science

Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

Prostate cancer is a significant public health concern, as it is the second most diagnosed cancer among men worldwide and it is one of the leading causes of cancer-related deaths among men. The goal of this project is to analyze and combine publicly available epigenomic markers data, transcription factor data and Hi-C data to identify genomic regions that differ between prostate cancer cell lines and normal cell lines. Our analysis involves comparing the epigenetic and Hi-C data of the three cell lines using graph embedding and page rank methods and identifying regions that show differential patterns using the transcription factor data. We hope that this work has the potential to contribute to a better understanding of the genomic differences underlying prostate cancer and can lead to the development of new therapeutic strategies.

#45 Investigating the role of extracellular matrix aging in tumor cell adhesion to 3D-scaffolds

Anupom Deb Nath and Stefan W. Vetter

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Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

Extracellular matrix (ECM) plays a critical role in both cellular homeostasis, and tumor growth and metastasis. Aged or glycated ECMs are better mimics of cancer cell growth substrate compared to non-aged ECM. Our study suggests that glycated collagen influences cell spreading area, eccentricity, as well as cell motility and migration. These changes in cellular behavior certainly regulate cancer cell adhesion and proliferation. That is why aged ECM are better *in-vitro* model systems to evaluate novel cancer therapeutics.

#46 Investigation of Adhesion Forces on the Surface of Borrelia burgdorferi using AFM

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Sponsor(s): ND ACES Emerging Seed Award UND0027590 and NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

The Lyme disease spirochete, *Borrelia burgdorferi* (Bb), is the leading cause of arthropod-borne disease in the USA. Adhesion is important to the establishment of infection and contributes to dissemination, persistence, and immune evasion. Therefore, understanding bacterial adhesion at the molecular level is crucial. Atomic Force Microscopy (AFM) can provide both the topography and mechanical properties of biological samples. With AFM, we measured adhesive forces between AFM tips and adhesins on the surface of live Bb.

#47 Laser Wireless Powering and Beam Tracking *via* Photovoltaic Array

Ahmed Elfarran and Bo Liang

University of North Dakota, School of Electrical Engineering and Computer Science, College of Engineering and Mines

Here we present a new system combining a 4-quadrant photovoltaic array, feedback control system, and laser source enables real-time laser tracking on a moving target while providing power to the laser. Its accuracy and performance were tested across various PV cells with 1W max power. This system has potential for various applications such as drones, biomedical, and industrial manufacturing, improving efficiency and accuracy of laser-based processes while minimizing energy consumption.

#48 Machine learning approaches for classifying temporal patterns and tracing causality in RNA-Seq datasets

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University of North Dakota, Department of Physics and Astrophysics and Department of Biology

Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

In an organism, how a cell-fate choice is made, during which genes are expressed differently, is yet to be understood. Decoding gene regulatory networks is important in understanding cell-fate choice, and hematopoiesis, is a good model to study cell-fate choice. In this project, we will analyze a genome-wide RNA-Seq time series dataset using non-negative matrix factorization (NMF), which is an unsupervised machine learning technique. Future work will identify metagenes that are expressed at particular times.

#49 Mentoring Early Career Teachers and Supporting North Dakota Schools through the Rural Student Teaching Experience: Participant Profiles from Fall 2021 to Spring 2023

Maria Zaman, Jill Baird, Naomi McGaughey, and Ryan Summers

University of North Dakota

Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1355466

The ND-ACES Rural Student Teaching Experience (RSTE) provides early career teachers with mentorship and support while they are placed in small schools and communities in North Dakota. The mentorship program is designed to encourage self-reflection and help induct new teachers into the profession. Prior research has identified mentoring as an effective strategy for helping early career teachers transition into their new classroom, school, and community. It may also help retain them in the profession. Since the program started in Fall 2021, five early career teachers have participated in the program. All of these individuals are still teaching across the state as of Spring 2023. This poster summarizes these activities of the RSTE program to date, and shares profiles of the early career teachers who have participated in the program.

#50 Multifunctional Applications of MXenes in Bone Mimetic Nanoclay Scaffolds

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Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

MXenes with their intriguing properties such as high conductivity, hydrophilicity, and biocompatibility have emerged as an attractive material for multifunctional applications. In this study, we focus on Ti_3C_2 MXene in bone mimetic nanoclay scaffolds, in which nanoclay scaffolds were proven to be a reliable 3D model for mimicking bone microenvironment of bone metastatic cancer and also bone regeneration. A combination of MXene and nanoclay scaffolds can present potential applications in biosensing, metastasis testbed models, and bone transplantation.

#51 Multifunctional Nanoparticles for Synergistic Photodynamic/Photothermal Therapy

Yingfen Wu, Xu Wu, Diane C Darland, and Julia Xiaojun Zhao

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Sponsor(s): NSF grant CHE 1709160, NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202, and NIH COBRE 2P20GM104360-06A1

To improve the therapeutic efficiency of Photodynamic/Photothermal Therapy (PDT/PTT), poly (styrene-co-maleic anhydride) (PSMA) was used as a crosslinker to incorporate Mn ions which could produce O_2 by H_2O_2 catalysis to reverse the tumor hypoxia and thus improving the therapeutic efficiency of PDT, poly [2,6-(4,4-bis (2-ethylhexyl)-4H-cyclopenta [2,1-b;3,4-b′] dithiophene)-alt-4,7-(2,1,3-benzothiadiazole)] (PCPDTBT) was used as a photosensitizer to trigger PDT/PTT. The synthesized Pdots showed great potential to improve synergistic PDT/PTT efficiency for cancer therapy.

#52 Multiscale Modeling of Nanocellulose Network Towards Understanding the Mechanical Performance

Zhaofan Li, Yangchao Liao, and Wenjie Xia

North Dakota State University, Department of Civil, Construction and Environmental Engineering

Sponsor(s): NSF CMMI Award 2113558 and ND EPSCoR New Faculty Award

Cellulose nanocrystals (CNCs) draw considerable interest in engineering and technological applications due to their excellent mechanical and physical properties associated with dynamic and microstructural features. Here, we present a coarse-grained (CG) modeling study for investigations of mechanical performance of CNCs bulk material forming a porous network microstructure, and how the dynamics and microstructure change in the CNC films under tensile deformation, aiding in the tailored design of cellulose-based materials for their mechanical performance.

#53 National Lakes Assessment (NLA) 2022: North Dakota's Lake Water Quality Assessment

Innocent K. Anosike and Yeo Howe Lim

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Sponsor(s): ND EPSCoR

In the United States of America, there are over 20,000 lakes, ponds, reservoirs, and wetlands which are studied under the National Lakes Assessment (NLA) and categorized under the U.S. Environmental Protection Agency (USEPA) as Watershed Program Management. In North Dakota, lakes are part of the surface water quality assessments, which is very important to the government, environmental engineers/scientists, natural resources professionals, public health experts, and North Dakotans in general because, the abundant surface water serves as drinking water sources, wildlife ecosystem balance, and fishery sustainability. North Dakota has over 400 lakes, but the State Government (including, Department of Environmental Quality, and Department of Water Resources) recognizes 247 lakes and reservoirs for surface water quality assessments in the state. Of these 247 lakes, 139 are man-made reservoirs, and 108 are natural lakes.

From surface water assessment database for North Dakota, the 139 reservoirs have an aerial surface of 543,156 acres, of which 480,731 acres or 63% of the state's entire surface water and reservoir acres are contained within the two mainstream Missouri River reservoirs (Lake Sakakawea and Lake Oahe). The 108 natural lakes in North Dakota cover 218,518 acres, with approximately 117,697 acres or 54% attributed to Devils' Lake. In North Dakota, there is an estimated 3 million acres of wetlands, whose majority are temporary, seasonal, semi-permanent and permanent depressional wetlands located in the Prairie Pothole Region. This research will boost drinking water quality, statistical computation on surface water assessments for drinking water in North Dakota, drinking water assessments viability on surface water resources, non-point water source management decisions, North Dakota watershed restoration and conservation, and the need for additional parameters on water informatics in North Dakota.

#54 Numerical Simulations of Leukocyte Rolling in Microchannel

Tam T. Nguyen, Lahcen Akerkouch, Amit Joshi, Benjamin Gantner, and Trung B. Le

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Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

Rolling of White Blood Cell (WBC) on endothelial wall plays a vital role in the human immune system. In this work, we replicate the process of WBC rolling in blood flow in microchannels. The WBC is assumed to have an initial shape of idealized sphere. The computational modeling of WBC transportation in fluid flows is simulated using fluid-structure interaction. Dissipative Particle Dynamics is used to model the cellular dynamics of membrane and cytosol.

#55 Optimization of *in vitro* 3D spheroid models of melanoma for anti-melanoma drug study

Yousuf Alam and Estelle Leclerc

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Sponsor(s): NIH DaCCoTA Center NIGMS U54 GM128729 and NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

Activation of the receptor for advanced glycation end product (RAGE) promotes tumor growth and chemoresistance. We describe here the optimization of 3D cell culture models of melanoma tumors that would allow investigating the role of RAGE in chemoresistance without the use of animal models.

#56 Passive Propulsion of Cells in Pulsatile Flows

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Sponsor(s): National Institute of General Medical Sciences NIH grant 8 P20 GM103442-12, NSF ND EPSCoR OIA-1946202, Extreme Science and Engineering Discovery Environment allocation CTS200012, and a start-up package of Trung Le from North Dakota State University

The passive propulsion of red blood cells (RBCs) and cancer cells in pulsatile flows is an area of active research that has garnered significant attention in recent years. Pulsatile flows are a common feature of many biological systems, and the ability of cells to navigate these flows is critical for their proper function. This study involved simulating the dynamics of a single RBC and a realistic cancer cell, which was based on in-vitro confocal scans. The cellular dynamics was modeled using a hybrid continuum- particle approach, wherein the Dissipative Particle Dynamics was employed to simulate the cellular dynamics and the Immersed Boundary Method was used to model the extracellular flow. This approach facilitated the efficient simulation of fluid flows in complex vasculatures. Our results, showed the unique extracellular flow patterns induced by the cellular dynamics of the RBC and the cancer cell when subjected to steady and pulsatile flow profiles.

#57 Photoluminescence of Single-Walled Carbon Nanotubes with Di-valent sp3 defects

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Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

Semiconducting single-walled carbon nanotubes (SWCNTs) are appealing candidates for applications such as single-photon emission and high-contrast bio-imaging. SWCNTs low emission yield due to low-lying optically forbidden states. Introducing sp^3 quantum defects in the sidewalls of SWCNTs through covalent functionalization is an excellent route to predictably modify nanotubes optical, electronic structures and develop advanced optoelectronic functionality. In aryl functionalized SWCNTs, the binding configurations of the aryl group define the energies of the emitting photons[1]. Insights into correlations between optical and structural properties of SWCNTs with chemical defects are important for controlling and tuning their emission. Here, we explore protocol to control chemical binding configurations of quantum defects on SWCNTs also referred as organic color centers through the photoexcited states. Simulations were performed to optimize the N-methyl-di-oxy-pyrrole functionalized SWCNTs (11,0) and (10,0) at three different ortho binding configurations (O++, O+ and O-). Density functional theory (DFT) calculations were performed using VASP with the generalized gradient approximation (GGA) Perdew−Burke−Ernzerhof (PBE) functional in a plane-wave basis set along with projector augmented-wave (PAW) pseudopotentials. For approximate evaluation of optical spectra, the oscillator strengths for HOMO-LUMO transitions were obtained by adopting independent orbital approximations. Non-adiabatic calculations are performed to allow dissipation of energy from electronic to nuclear degree of freedom to explore non-radiative relaxation of excited states.

The outcome of controlled chemical functionalization in the SWCNTs activates the red-shifted photoluminescence with longer lifetimes and higher photoluminescence yield. These findings impact a variety of practical applications of doped nanotubes as quantum light sources for quantum information technologies that can also be expanded to controlled chemical functionalization of any nanomaterials.

We correlated our results with different experimental studies to better understand the opto-electronic behavior of defect-states of functionalized CNTs.

#58 Plant Polymer Arabinoxylan Based Soft Scaffolds for Breast Cancer Cell Growth and Proliferation

Md Sultan Mahmud, Brooke Roeges, Haley Boechler, Kaydee Koistinen, Julia Kohl, Trevor Gravseth, Alize Pratt, Caden Bjornstad, Michael Kjelland, and Khwaja Hossain

Mayville State University

Sponsor(s): ND EPSCoR

Biopolymers are functional material; major portion of biopolymers are derived from plants which are of great interest to researchers and professionals across various disciplines. The bioactive materials have the capability of affecting biological surrounding and biomaterial-based scaffolds have traditionally been used to provide a bioactive environment in which cells adhere and proliferate. We are working on developing soft scaffolds prepared with various types of polymers which can support cancer cell growth and proliferation.

#59 Poly(silyl ether)-Based Nanoparticles for Use as Potential Nanocarrier

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Sponsor(s): NSF ND EPSCoR Track 1 Cooperative Agreement OIA-1946202

Polymeric nanoparticles present a method of cancer treatment through the selective targeting and controlled release of drugs. Poly(silyl ether)'s (PSEs) based nanoparticles show promising use due to the hydrolytic degradation of the Si-O-C bond present in the molecule. In the current study, we have prepared and characterized a series of PSEs from polyethylene glycol (PEG) based diols and PSEs-based nanoparticles. The encapsulation and subsequent release of payload by these nanoparticles are being studied and optimized.

#60 Precipitation analysis before flood events that breakdown highway H191 Montana

Daniel Iancu and Yeo Howe Lim

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Sponsor(s): ND EPSCoR

Mobridge Slide is a section of highway US 191 that experiences continual breakdown and washout resulting from hydrologic issues. The proposed project objective is to analyze the hydrological data from the site area to determine the precipitation values that lead to multiple breakdowns of the highway. Statistical analysis will be used to assess historical recordings prior to highway failures. The importance of this study could be applied to other similar areas with highways that connects communities affected by floods.

#61 Quantitatively Evaluation of single-cell Hi-C Imputation and Smoothing Methods

Bin Zhao and Lu Liu

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Sponsor(s): National Federation EPSCoR Track-1 Cooperative Agreement OIA-1946202

There are many imputation methods for coping with the sparseness issue in single-cell Hi-C (scHi-C) data. They impute the original contact matrix in single cells by forming hypergraphs, using Bayesian Estimates or transformation so that the contact matrix would be denser and more information would be obtained for further investigation. We evaluated ten imputation and smoothing methods on their capacity of TAD-like boundaries calling, significant chromatin interactions calling, and cell embedding learning. We also measured the impact of the change in cell similarity on those capacities. We justified our conjecture by comparing the results of imputed ones with the raw data using several evaluation tools and metrics.

#62 Quantum Mechanical Treatment of Cancer Cell Adhesion

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Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

Quantum Mechanics (QM), utilizes the wave- or electron density function in the Schrodinger equation, can produce reliable models in various systems unlike Classical Mechanics. A key system under investigation is cancer cell migration, which occurs due to trans-proteins on the cancer cell's surface, named αvβ3 integrin, binding to Arginylglycylaspartic acid (RGD) sequences in the Extra Cellular Matrix. The goal of the research is to perform QM calculations to produce a reliable model of integrin-RGD binding.

#63 Salts Removal as an Effective and Economical Method of Bakken For Oilfield Produced Water Treatment

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Produced water in the unconventional U.S. Bakken oilfield has become a significant concern since oil and gas production growth has been substantial, and operating costs are increasing. Reusing this considerable amount of produced water has become necessary since the treated water can be used for potable supplies, irrigation, deep well injection, maintenance, and fracking, which improves profits and mitigates groundwater pollution. The total dissolved solids (TDS) in the ND Bakken formation are greater than 300g/l, which is much higher than the concentration of salt in seawater; therefore, it is reasonable to propose selective precipitation to treat the salts found in this formation's produced water. Extracted salts are effective coagulants for removing various contaminants from wastewater. We will extract several metals (Mg, Ca, Mn, Sr, Li, and K) from the flowback water and water produced in the Bakken oilfield using lime and soda ash at different dosages and pH values during this project. The separation treatment using selective precipitation can be invaluable as a pre-treatment process of desalination techniques. Additionally, the extracted $Mg(OH)_2$ and $CaCO_3$ will be used for wastewater treatment and establish their efficiency in removing COD and the nutrients phosphorous and nitrogen from ND wastewater.

#64 Screening of Phytochemical-enriched Plant Extracts against Bone Metastatic Breast Cancer grown on 3D *in vitro* Nano-clay based Bone-mimetic Scaffold

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Sponsor(s): North Dakota State University Center for Engineered Cancer Testbeds and NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

Phytochemical-enriched plant extracts contain vast array of phytochemicals which have numerous health benefits. Bone metastatic breast cancer is a fatal disease in which many of the available anticancer therapeutics are ineffective due to lack of accurate drug screening models. In this study, we screened three plant-extracts on our 3D *in vitro* model of breast cancer bone metastasis. We have performed various experiment to observe their cytotoxicity to both bone metastatic breast cancer and bone cells.

#65 Single ligand-receptor binding spectroscopy of cancer biomarkers

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Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

In this study, we employed single-molecule binding force spectroscopy to investigate the binding and unbinding forces between several membrane receptors on tumor-derived exosomes and their respective ligands. We compared the surface density of these receptors on the exosomes and their binding strength to the ligands. Our results show that each ligand-receptor interaction remains consistent across all exosomes isolated from healthy, non-metastatic, and metastatic cancer cell lines, but the surface density of receptors varies.

#66 Smart Earth Station Antenna for Satellite IoT Communications

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Sponsor(s): ND EPSCoR seed funding

Numerous enterprises require to deploy assets in remote places due to the services and applications they provide. Satellite communication can offer a reliable solution for remote connectivity between IoT devices where there is no or limited access. A novel single element planar antenna has been designed for bidirectional-communication with moving-LEO-satellites in C-band. Based on link-budget calculation and the measured gain of the antenna, the required number of elements were determined to incorporate into an array.

#67 Sustainable Management of Dams and Reservoirs in North Dakota: Sediment Transport Characterization

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Selected reservoirs in the state of North Dakota would be surveyed to assess their storage capacity and the dynamics of sedimentation. The HYCAT, a multi-sensor autonomous surface vehicle that would be used, simultaneously measures water quality, velocity, flow and depth, and acquires high quality bathymetry data. The data would be compared to previous surveys to establish a time series analysis of the reservoir bathymetry. This would inform further discussion on the suitability of each reservoir to perform its functions. Recommendation shall be given on the most suitable sediment management method for the dam downstream based on the sediment characteristics, and the water properties.

#68 SWAT Modeling: Influences of Land Use and Land Cover on Streamflow and Water Quality

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Sponsor(s): Environmental Protection Agency Project FAR0035144

Watershed modeling relies heavily on land-use land-cover (LULC) data, so selecting accurate LULC is crucial. The objective of this study is to demonstrate the effect of different LULCs on hydrologic processes and nutrient loading of a watershed. To assess the impact, two different LULC datasets were used in the modeling of the Soil and Water Assessment Tool (SWAT). The findings of the study offer important guidance for selecting the right LULC data for watershed modeling.

#69 Synergistic anticancer effects of two drug combinations on pancreatic ductal adenocarcinoma cell lines

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Sponsor(s): NIH grant 2 R01GM 114080, NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202, and NIH DaCCoTA Center NIGMS U54 GM128729

Pancreatic ductal adenocarcinoma is a fatal disease with a poor prognosis, necessitating the urgent need to develop new therapeutic strategies. Hypoxia is a significant characteristic of solid tumors. Hypoxia increases pancreatic cancer progression, metastasis and reduces the effectiveness of chemotherapy. We encapsulated an anticancer drug (gemcitabine) and a CXCR4 receptor antagonist (plerixafor) in bilayer vesicles prepared from amphiphilic block copolymers. The synergistic combination of gemcitabine and plerixafor showed increased potency in hypoxia compared to normoxia.

#70 Synergistic drug combinations to kill triple-negative breast cancer cells

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Sponsor(s): NIH grant 2 R01GM 114080, NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202, and NIH DaCCoTA Center NIGMS U54 GM128729

Hypoxia in triple-negative breast tumors increases invasiveness and poor patient outcomes. Drug delivery systems limit anticancer drugs' harmful side effects in required concentrations. Sulfasalazine was conjugated to polymer nanoparticles for active targeting to the overexpressed SLC7A11 receptors on triple-negative breast cancer cells under hypoxia. The nanoparticles encapsulated the drugs doxorubicin and metformin. A combination of the two drugs synergistically killed the triple-negative breast cancer cells in hypoxia.

#71 Synergistic Treatment of Triple-Negative Breast Cancer Using Encapsulated Drugs

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Sponsor(s): NIH grant 2 R01GM 114080, NSF EPSCoR Track-1 Cooperative Agreement OIA-1946202, and NIH DaCCoTA Center NIGMS U54 GM128729

Triple-negative breast cancer (TNBC) is challenging to treat, lacking the estrogen receptor, progesterone receptor, and HER2 protein expressions. In addition, TNBC tumors are aggressive and fast-growing, causing hypoxic or low-oxygen regions to form. These regions contain more cancer stem cells making treatment increasingly difficult. By using hypoxia-sensitive polymersomes to encapsulate all-trans retinoic acid to reduce stemness and doxorubicin to kill the cells, we plan to treat TNBC tumors better.

#72 Synthesis and Characterization of Degradable Hyperbranched Poly(silyl ether)

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Sponsor(s): NSF ND EPSCoR Track 1 Cooperative Agreement OIA-1946202

Hyperbranched polymers are a class of polymers that can be synthesized with no byproducts and controlled degree of branching. The introduction of further functional groups allows researchers to attach drugs and targeting agents directly to the polymers. Silyl ether functionality is known to degrade under mildly acidic or basic conditions found in the human body. Here we describe the synthesis of hyperbranched poly(silyl ether)s by a classical A2+B3 approach from hydrosilanes and diols. The obtained polymers can be further made into nanoparticles for drug loading and targeted release of drugs in cancer cells.

#73 Synthesis and Characterization of SLIT3-releasing PLGA/hydroxyapatite scaffold via indirect 3D printing for Bone Tissue Engineering

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Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

Three-dimensional printing technology offers flexible design possibilities, precise geometrical control, and feasible surface modification; however, direct 3D printing employs a limited number of biomaterials and structures which restricts the opportunities needed for the bone extracellular matrix mimicking. In this work, the indirect 3D printing technique was utilized to produce hierarchically porous slit3-releasing PLGA/hydroxyapatite nanocomposite coated with polydopamine (PLGA-HA,NPs-PDA) scaffold. the Slit3 protein efficacy toward cell growth in polymeric scaffold matrix had been addressed for the first time. The characterization results have promising prospects with application of the scaffold for bone tissue regeneration.

#74 Synthesis of Highly Selective Fluoroionophore for Selected Metal Cations and Their Biological Applications

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Sponsor(s): ND EPSCoR

This work outlines the synthesis of MC 25 [15 Crown –5] which is a metal ion selective ionophore. The synthesis proceeds in four steps: begin with DMN synthesis followed by hydrogenation to prepare DMA, then synthesis of OEG6DTs, and finally the formation of the macrocyclic ring structure from DMA and OEG6DTs which is confirmed by ^{1}H NMR spectroscopy. Combining MC 25 with a fluorophore makes fluoroionophore that will be used for clinical diagnostics.

#75 Targeting TNBC tumors using hypoxia responsive nanoparticles containing drugs with a synergistic effect.

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Sponsor(s): NIH grant 2 R01GM 114080, NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202, National Institute of General Medical Sciences NIH grant 8 P20 GM103442-12, and NIH DaCCoTA Center NIGMS U54 GM128729

Triple-negative breast cancer (TNBC) is an aggressive disease, and lacks the expressions of estrogen, progesterone, and HER2 receptors. Limited response to hormonal and immune therapies makes it difficult to treat. We found that the anticancer drug doxorubicin and the stemness inhibitor Napabucasin synergistically regulate the proliferation of metastatic TNBC cells in Normoxia and hypoxia. We hypothesize that combination treatment of the two drugs encapsulated in polymersomes will produce significant reduction in TNBC tumor size.

#76 The Optimization of Spin-Dependent Optical Properties of Mo(0) Complexes

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Sponsor(s): Department of Energy Grant DE-SC0022239, NSF MRI Award 2019077, and ND EPSCoR

Transition-metal complexes (TMCs) have shown a great promise in design of optically addressable qubit candidates for quantum information science. To realize optical initialization and read-out signals, TMCs must have a triplet ground state and have the lowest lying excited state be a singlet that decays to triplet ground state. The goal of this research is to establish the relationship between excited properties and chemical structure of Mo(0) complexes using density functional theory.

#77 Towards Artificial Intelligence (AI) Equipped Smart Antenna system for Satellite-Based Internet of Things (IoT)

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North Dakota State University, RF-Connect Lab

Sponsor(s): NSF ND EPSCoR seed funding

Satellite-based IoT services are reliable for remote connectivity, but bidirectional communication with LEO satellites is unavailable. This project proposes a phase array antenna system for earth station which is able to sustain communication with moving LEO satellites. In view of this, a single element antenna is designed, and a novel link budget calculation is performed that offers simple addition (subtraction) of required number of elements to (from) the proposed array.

#78 Unraveling Integrins' Conformational Changes and Mechanics at the Molecular Scale

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Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

The integrin is the cell surface protein, couples the extracellular matrix (ECM) to the cell cytoskeleton. In this study, steered molecular dynamics simulations is used to investigate the mechanical responses of fibronectin bound integrin αvβ3. The results indicate that fibronectin ligand binding modulates the mechanical responses of integrin in the folded and unfolded conformation states during forced deformation. These findings contribute to understanding the mechanotransmission between cells and extracellular matrix, providing new insights into integrin-mediated adhesion.

#79 Using NVIDIA Omniverse Technology to Better Convey the Concepts Demonstrated by Computational Fluid Dynamics Simulations

Njiru Mwaura and Aaron Bergstrom

University of North Dakota

Sponsor(s): NSF ND EPSCoR Track-1 Cooperative Agreement OIA-1946202

The study conducted used Omniverse, NVIDIA Corporations new metaverse digital twin technology, to visually enhance data extracted from a Paraview model of a human blood cell moving through a simulated fluid. This research utilized CFD data originally developed by Dr. Akerkouch and Dr. Le at NDSU under the project ND-ACES cancer research. Omniverse was explored for applications in simulations and animations due to its versatility as compared to the usual Computational Fluid Dynamics applications.

The aim of this study is to offer 3D visualizations and simulations of accurate, AI-enabled, virtual simulations that are perfectly synchronized with the real world. The overall objective of using Omniverse as a simulation tool is to produce digital twins for transforming industries and scientific discovery, as well as delivering superpowers to developers, researchers, and enterprises who use them to design, simulate, and optimize products, equipment, and processes in real-time, before ever going to production.

This research entails porting the content to interactive VR environments for research and education in a learning institution setup. In addition, the research project would like to leverage the Digital Twin capabilities of Omnivese, so that robust AI CFD could be done directly inside Omniverse platforms.

#80 Valorization Of North Dakota's Corn Mill Waste Stream and Its Application in Corrosion Inhibition

Olufemi Oni, Isra Elsamani, and Yun Ji

University of North Dakota, Department of Chemical Engineering

Sponsor(s): ND EPSCoR and North Dakota Corn Council

Agricultural products' waste streams pose a great threat to human environment especially the waste stream fermented by Bacillus spp. in corn wet milling industries called the corn steep liquor. These microorganisms secrete secondary metabolites suspected to contain surface-active compounds. In this study, the biosurfactant was extracted at 60^{o}C using liquid-liquid extraction. Its application in corrosion inhibition of mild steel was investigated at concentrations of 0, 0.01, 0.02 and 0.03 g/ml at 30^{o}C in saline environment.

Post-Doctorate Students and Faculty

#81 Defect Process in MAB Phase

Salawu Omotayo Akande and Deniz Cakir

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Sponsor(s): Air Force Office of Scientific Research

MAB phases have emerged as candidates for several applications due to the impeccable properties associated with them. To widen applicability, there is a need to understand the defect formation processes since knowledge from such investigations can be utilized in the design of resilient materials. By employing density functional theory (DFT) calculations, we identified the stability and the mobility of the most prominent point and extended defects in the MAlB (M=Mo and W) and N_2AlB_2 (where N= Cr and Fe) MAB phases under different chemical conditions.

#82 In-medium similarity renormalization group approach to atomic ions

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University of North Dakota, Department of Chemistry

Sponsor(s): National Science Foundation Grant OIA 1355466 and ND EPSCoR

In-medium similarity renormalization group method has expanded from theoretical nuclear physics to quantum chemistry as a new tool, since it may have an opportunity to enable precise theoretical calculations in relatively cheap way. We employ this technique to study properties of many-electron systems. Ground state energies for closed-shell light atomic ions are obtained from this approach and are in reasonable agreement with values from other approach and close to benchmark values in the literature.

#83 Exploring Singlet-Triplet Excitonic Properties in Aryl Functionalized (11,0) Single Walled Carbon Nanotube (SWCNT)

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North Dakota State University, Department of Chemistry and Biochemistry

Sponsor(s): Department of Energy EPSCoR grant-0814442; ND EPSCoR

The single-walled carbon nanotubes (SWCNTs) chemically functionalized by organic molecules has attracted recent attention because of their promising applications in optoelectronics, telecommunications, and quantum technology. Chemical functionalization provides the sp^3-defect at the tube surface resulting in an optically active lowest energy exciton, which is localized around the defect site. Here, we investigate the properties of singlet (S_1) and triplet (T_1) excited states in (11,0) zigzag SWCNTs using the plane wave basis set density functional theory (DFT). The sp^3-defect in the sp^2-carbon lattice of the nanotube is created through covalent attachment of aryl with various electron withdrawing (EW), electron donating (ED), and neutral (N) groups: $R = NO_2, NH_2$, and H. The excitonic state was calculated using non-equilibrium population of the lowest unoccupied orbital (LUMO) creating excited electron-hole pair. Obtained results reveal the fact that the optically active states that corresponds to various ortho (O) and para (P) defects redshifted from the main optical band E_{11} of the pristine nanotube. The order of the redshift (ΔE_{BS}) based on different functional group is: $C_6H_4NO_2$ > C_6H_5 > $C_6H_5NH_2$ corresponding to the most localized defect. Our calculations also show that higher the value of singlet-triplet energy gap (ΔE_{ST}) higher is the value of ΔE_{BS} and vice-versa. Also, the value of (ΔE_{ST}) and (ΔE_{BS}) are more pronounced with B3LYP than PBE functional explaining B3LYP functional provides more accurate optical properties than PBE. Our results provide better conditions for populating the triplet state and making it promising for optically accessible molecular qubits.

#84 Theoretical Prediction of stable quaternary phases by Transition Metal Doping in orthorhombic-MoAlB Phase by the First-Principles Calculation: Is Doping always good?

Bipasa Samanta and Deniz Cakir

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Sponsor(s): Air Force Office of Scientific Research

First principle Calculations is carried out to explore the phase stability of orthorhombic MoAlB phases by doping transition metal (TM) in place of Mo. The predicted quaternary phases are found to be stable in-terms of formation energy for few TM. Latter we try to characterize the property of the quaternary phases based on electronic, thermal, and mechanical property and try to draw a trend based on the atomic property of TM used.

#85 Rocks and Minerals – a Library of 3-dimensional Images

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Sponsor(s): FY23 STEM Award

Rocks and Minerals is a digital photogrammetry database hosted by sketchfab.com at https://sketchfab.com/rocksandminerals. The database contains nearly 600 three-dimensional models of rock and mineral specimens. These models are easily accessed for free via the web. Much of our initial work focused on museum-quality mineral and rock samples but we are now populating the database with more common specimens.

Many of our models are beautiful and captivating because they allow rotation and zoom-in capabilities, permitting specimens to be viewed down to sub-millimeter scale. Thus teachers and students can examine rocks and minerals in 3-d and can look at details and properties that otherwise would be difficult to discern. We find the models to be especially useful for looking at mineral properties such as cleavage and habit. And, rock properties such as crystallinity and the relationships between different mineral constituents are much more easily seen than with traditional photographs. Our models also may be used as part of virtual field experiences.

Notes

Notes


ND EPSCoR
CCBSE - Cellular
CCBSE - Computation
CCBSE - Materials
PROSPER
NSF