ND EPSCoR

2022 STATE CONFERENCE

ALERUS CENTER
GRAND FORKS, NORTH DAKOTA
WEDNESDAY, APRIL 6, 2022

Hybrid ND EPSCoR 2022 State Conference Agenda
Wednesday, April 6, 2022
Alerus Center – 1200 South 42nd Street – Grand Forks, ND

7:30 am – 8:30 am CDT

Registration, poster set-up and viewing, and breakfast. The posters are available for viewing all day.

8:30 am – 10:00 am CDT
Ballroom

Welcome

8:30 am – 8:37 am CDT – Dr. Kelly A. Rusch, Executive Director of the ND EPSCoR State Office and NSF Track-1 Principal Investigator/Project Director

Welcome from North Dakota University System

8:37 am – 8:45 am CDT – Jerry Rostad, Vice Chancellor for Strategy and Strategic Engagement, North Dakota University System

Welcome from ND Congressional Delegation

8:45 am – 8:50 am CDT – Tom Brusegaard, Staff Representative, on behalf of Honorable John Hoeven, United States Senator

8:50 am – 8:55 am CDT – Randy Richards, Staff Representative, on behalf of Honorable Kevin Cramer, United States Senator

8:55 am – 9:00 am CDT – Mary Christy, Staff Representative, on behalf of Honorable Kelly Armstrong, United States Representative

NSF Perspective

9:00 am – 9:20 am CDT – Dr. Sandra Richardson, NSF EPSCoR Section Head

9:20 am – 10:00 am CDT – Dr. Jose Colom-Ustariz, NSF EPSCoR Program Officer for ND EPSCoR RII Track-1 ND-ACES Cooperative Agreement

10:00 am – 11:00 am CDT
Ballroom

ND-ACES

Moderators: Dr. Archana Dhasarathy (UND; Biomedical Sciences) and Dr. Sanku Mallik (NDSU; Pharmaceutical Sciences)

10:05 am – 10:15 am CDT – Dr. Kalpana S. Katti (NDSU; Civil, Construction and Environmental Engineering)

10:20 am – 10:25 am CDT – Dr. Sarah Sletten (UND; Biomedical Sciences)

10:30 am – 10:40 am CDT – Dr. Hilde van Gijssel (VCSU; Science)

10:45 am – 10:50 am CDT – Nicholas Bittner (CCCC; Engineering); Advisors: Dr. Brent Voels (CCCC; Science) and Michael Parker (CCCC; Pre-Engineering/Math)

10:50 am – 11:00 am CDT – Dr. Binglin Sui (UND; Chemistry)

11:00 am – 12:00 pm CDT
Ballroom

ND-ACES Poster Session Hybrid Q&A
Moderators: Dr. Colin K. Combs (UND; Biomedical Sciences), and Dr. Kalpana S. Katti (NDSU; Civil, Construction and Environmental Engineering)
11:00 am – 12:00 pm

12:00 pm – 1:00 pm CDT
Ballroom

Lunch Keynote Speaker – Dr. Candan Tamerler, ND-ACES EAB Chair
Introduction: Dr. Kelly A. Rusch, Executive Director of the ND EPSCoR State Office and NSF Track-1 Principal Investigator/Project Director
Speaker: Dr. Candan Tamerler, Associate Dean of Research, School of Engineering, Wesley G. Cramer Professor, Department of Mechanical Engineering, University of Kansas
12:15 pm – 1:00 pm CDT

1:00 pm – 2:00 pm CDT
Ballroom

Annual STEM-based Indigenous Knowledge and Research Panel
Moderator: Raymond Burns, Tribal Partnerships Manager, ND EPSCoR
Speakers: Dr. Shelly Valdez, President of Native Pathways; and Jill Stein, Principal Consultant at JKS Consulting

1:00 pm – 2:00 pm CDT

2:00 pm – 3:00 pm CDT
Ballroom

Panel on Industry Partnerships
Moderator: Dr. John Mihelich, Interim Vice President for Research & Economic Development, UND
Speakers: Dr. Sinan Keten, Professor of Mechanical Engineering and Civil and Environmental Engineering and (by courtesy) Biomedical Engineering, June and Donald Brewer Professor, Northwestern University; Dr. James Brown, CEO and President, Agathos Biologics; and Dr. David Pearce, President of Innovation and Research, Sanford Research
2:00 pm – 3:00 pm CDT

3:00 pm – 4:00 pm CDT
Ballroom

ND-ACES
Moderators: Dr. Dinesh R. Katti (NDSU; Civil, Construction and Environmental Engineering) and Dr. Julia Xiaojun Zhao (UND; Chemistry)

3:05 pm – 3:15 pm CDT – Dr. Mark Hoffmann (UND; Chemistry)
3:20 pm – 3:25 pm CDT – Brooke Roeges and Hayle Boechler, *previously recorded* (Mayville State University; Biology), Advisors: Dr. Khwaja G. Hossain (Mayville State University; Biology) and Dr. Michael E. Kjelland (Mayville State University; Biology)
3:30 pm – 3:40 pm CDT – Dr. John C. Wilkinson (NDSU; Chemistry and Biochemistry)
3:45 pm – 3:50 pm CDT – Lahcen Akerkouch (NDSU; Civil, Construction and Environmental Engineering), Advisor: Dr. Trung Bao Le (NDSU; Civil, Construction and

Environmental Engineering)
3:55 pm – 4:00 pm CDT – Dr. Colin K. Combs (UND; Biomedical Sciences)

4:00 pm – 4:30 pm CDT
Ballroom

Closing Remarks
4:00 pm – 4:30 pm CDT – Dr. Kelly A. Rusch, Executive Director of the ND EPSCoR State Office and NSF Track-1 Principal Investigator/Project Director

Abstract Booklet

Numbered posters will be displayed at the in person conference event at the Alerus Center in Grand Forks, ND. Posters without numbers are displayed virtually only.

Photography and Videography

All sessions of this hybrid conference are being recorded. Please contact cailin.shovkoplyas@ndus.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.

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

#1 **3D Bioprinting Using Human Cancer and Stem Cells with Novel Arabinoxylan Bioink for 3D Cell Culture**

Julia Kohls, Trevor Gravseth, Brooke Roeges, Hayle Boechler, Khwaja Hossain, Madisen Knudsvig, Michael Kjelland, Mayville State University, Division of Science & Mathematics

ND-ACES

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

Wheat bran constitutes about 15% of the wheat grain and contains large amounts of arabinoxylan (AX). The goal of the present research was to establish *in vitro* cultures of human mesenchymal stem cells and MiaPaca-2 cells, 2D and 3D, with and without AX and determine whether an AX bioink for 3D bioprinting could be an alternative to using commercial bioink, e.g., LifeInk200. Bioprinting was successful with LifeInk200 and will be tested with AX bioink next.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37753

#2 **3D In Vitro Model of Patient-derived Breast Cancer Cell line Mimic In Vivo Features**

Shrinwanti Ghosh, Farid Solaymani Mohammadi, Sangdeuk Ha, Jiha Kim, North Dakota State University, Department of Biological Sciences

ND-ACES

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

3D in vitro models have been applied in cancer research as a transitional model between in vitro cancer cell cultures and in vivo tumors. The aim of this study was to create reliable in vitro models with characteristics close to in vivo tumors. We explore a 3D model to evaluate the proliferation capacity of breast cancer cells derived from patients. We revealed 3D is a promising model to evaluate essential tumor stages, including epithelial-mesenchymal transition, programmed cell death apoptosis.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37315

#3 **A Coarse-Grained Model for the Mechanical Behavior of Na-Montmorillonite Clay**

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

ND-ACES

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

Montmorillonite (MMT) is a fine-grained clay mineral that has different applications in industry such as drug-delivery systems, catalyst supports, etc. The current study presents a Coarse-Grained (CG) Molecular Dynamics (MD) technique to develop a computationally efficient model of Na-MMT clay with a typical size. Using the “strain-energy conservation” approach, the force field parameters for the model are obtained and the developed model can well preserve in-plane tension, shear, and bending behaviors of atomistic counterparts.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37246

#4 **A comparison of Machine Learning/Deep learning algorithms for the classification and prediction of cancerous tumors**

Solene Bechelli, University of North Dakota, Department of Biomedical Engineering

ND-ACES

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

With cancers being one of the leading causes of death, research in this field has considerably increased over the past decades. One way to improve the recovery chances in patients is its early detection. Moreover, with the improvements of Machine Learning algorithms, the determination of early diagnosis is made easier. In this study, we compare the performance of different algorithms from Linear regression and classification tree to pre-trained models such as ResNet50 or VGG16. In addition, we develop our own Convolutional Neural Network. We show that in addition to a similar performance in terms of accuracy, our CNN model provides much faster prediction than the pre-trained models.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37319

#5 **Ab Initio investigation of understanding the interaction between nano-montmorillonite clay surface and amino acids.**

Warnakulasuriya Ashan Fernando, Mohammed Jabed, Mark Hoffmann, and Deniz Cakir, University of North Dakota, Department of Physics

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

The interaction of amino acids with clay minerals results in the formation of novel biomaterial nanocomposite systems, promising such as for bone tissue regeneration through osteogenesis. Therefore, an atomistic understanding of nano-clay interaction with biologically relevant materials is of great importance. In this respect, we investigated the interaction of 11 unnatural amino acids with Fe and Mg co-doped montmorillonite clay using density functional theory calculations.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37333

#6 **An ongoing approach to determining a 3D protocol for a TNBC cell line**

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

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

Breast cancer accounts for the most common form of cancer worldwide. The culture of cancer cells on a scaffold allows for the growth of tumor spheroids which best mimics the native environment of the tumor as they rely on the extracellular matrix intricately involved in breast cancer metastasis. We have established a protocol for culturing a triple negative breast cancer line (TNBC), MDA-MB-231, as scaffold-supported spheroids suitable for drug susceptibility screening.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37314

#7 **Baseline Data Report: Promoting Retention & STEM Success Through Research Training Groups**

Andrea Doyon, Georgia Paul, Adel Said, Niyeli Herrera, Rachel Navarro, and Sarah Sletten, University of North Dakota, Department of Counseling Psychology

ND-ACES
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 as future STEM researchers. During Year 1, participants completed a baseline survey pertaining to their professional/technical skills, self-efficacy, persistence intentions, and sense of belonging. Students also received monthly newsletters and were rewarded for participating in events via a digital badging process.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37292

#8 **Development of an *in vitro* cellular model using 3D spheroids of melanoma cells and fibroblasts to mimic *in vivo* mouse models of melanoma**

Yousuf Alam and Estelle Leclerc, North Dakota State University, Department of Pharmaceutical Sciences

ND-ACES

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202 and the College of Health Professions at NDSU

RAGE is a receptor involved in Alzheimer's disease, diabetes, and cancers. We have shown that activation of the RAGE signaling pathway leads to increased tumor cell survival and chemoresistance. We propose here to develop and optimize 3D cell culture models of melanoma that resemble melanoma tumors and would allow investigating the role of RAGE in chemoresistance without the use of animal models.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37343

#9 **Early cancer detection by cell-free chromatin and AI**

Motoki Takaku, Xusheng Wang, Kincaid Rowbotham, Sakuntha D. Gunarathna, Aerica Nagornyuk, University of North Dakota, Department of Biomedical Sciences

ND-ACES

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. It has been also shown that cfDNAs partially retain epigenetic information, such as DNA methylation and chromatin structures including nucleosomes. In this project, we aim to establish a computational tool to predict the primary origin of cancer.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37440

#10 **Education and Workforce Development (EWD); PROmoting Sustainable Partnerships in Education and Research (PROSPER): Early Career Faculty Baseline Survey**

Ben Gilbert, Adel Said, Niyeli Herrera, and Marcus Banks, University of North Dakota, Department of Counseling Psychology

ND-ACES

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

The current study aimed to collect baseline data from the ND-ACES early career faculty (ECF) in crucial growth areas and assess interest in career development opportunities. Nine ECF completed all measures. Results suggest that ECF endorsed being highly skilled and confident in professional skills, while also being most interested in professional development topics surrounding grant management and writing. ECF also reported an average sense of belonging at work and no intentions of seeking other employment.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37734

#11 **Efficiency and optimization of two parallel processing methods on Talon**

Joseph E. M. Robertson, David Apostal, and Aaron Bergstrom, University of North Dakota, Department of Chemistry and the Computational Research Center

ND-ACES

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

The multi-core efficiency of a custom Python-based Monte Carlo volume approximation simulation program and an existing quantum chemistry program, GAMESS-US, on Talon were investigated. It was found that "embarrassingly parallel" simulations, such as the Monte Carlo simulation, benefited greatly from parallelization, but that a higher number of cores did not significantly improve performance. Similarly, in GAMESS-US, it was found that efficiency did not significantly improve beyond initial parallelization and actually decrease beyond 30 cores.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37298

#12 **Establishing and characterizing patient-derived breast cancer cell lines**

Farid Solaymani Mohammadi, Shrinwanti Ghosh, Anu Gaba, Kalpana S. Katti, and Jiha Kim, North Dakota State University, Department of Biological Sciences

ND-ACES

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

Patient-derived cancer cell lines are irreplaceable resources in basic and translational cancer research. We attempted to develop stable patient-derived breast cancer cell lines in 2D culture system and using an optimized culturing condition. Once the cancer cells were isolated and expanded in culture, they were immunostained with CK19, EpCAM, and vimentin expression using immunocytochemistry. We further developed and monitored the established cell lines in terms of phenotype and genotype characteristics.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37332

#13 **Feasibility Study of Alginate, Hyaluronic Acid and Chitosan Based Biomimicking Hydrogel**

Md Rakib Hasan Khan, Raj Shankar Hazra, and Mohiuddin Quadir, North Dakota State University, Department of Coatings and Polymeric Materials

ND-ACES

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

Hydrogels are self-supporting water-swollen 3D viscoelastic networks. It allows the attachment and diffusion of cells and molecules. Therefore, it has drawn attention in biomedical applications such as wound healing, bone regeneration and cell therapeutics. In this study, we investigated the feasibility of hydrogel in terms of different material analyses, such as pH study, Rheology study, Nanoindentation study etc.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37341

#14 **Hierarchically Porous Slit3-releasing Composite Scaffold for Bone Tissue Engineering**

Abdulrahman M. Al-Shami, Jadyn Guidinger, and Ali S. Alshami, University of North Dakota, Department of Biomedical Engineering

ND-ACES

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

This research concerns developing novel three-dimensional, highly porous, and interconnective scaffolds with high osteogenesis and angiogenesis properties for bone tissue engineering. These scaffolds are fabricated using a combination of two fabrication methods, i.e., indirect 3D printing and solvent casting and particulate leaching method, to obtain two levels of pore sizes (~ 500 μm and < 100 μm). Also, Slit3 protein is incorporated into the scaffolds to provide better angiogenesis and osteogenesis performance.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37270

#15 **Interactions of amino acids on Fe-Mg doped montmorillonite clay surfaces and its implications for electro-magnetic and biomedical applications**

Steven Westra, Dinesh Threpa, and Svetlana Kilina, North Dakota State University, Department of Civil, Construction and Environmental Engineering

ND-ACES

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

Amino acids are the building block of proteins and are 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 have been modeled using density functional theory, we

are interested to study the interaction of amino acids at the surfaces of the Fe-Mg doped MMT clay mineral. The proposed amino acids are 5-Aminopentanoic acid, 2-Aminoheptandioic acid, and 2-Aminooctanoic acid.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37304

#16 **Interpreting Denoising Autoencoders**

Dharanidharan Arumugam, Ravi Kiran Yellavajjala, North Dakota State University, Department of Civil, Construction and Environmental Engineering

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

The goal of this study is to interpret denoising autoencoders by quantifying the importance of input pixels for image reconstruction. The attributions quantifying the importance of the pixel features are computed using an automatable gradient approach based on complex step perturbation. The pixel attributions of the images, in the end, are plotted in the form of saliency maps. Three sanity checks are introduced to verify the fidelity of the generated saliency maps.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37305

#17 **Interstitial Fluid Flows of Bones**

Lahcen Akerkouch, Trung Le, Berkay Koyuncu, Haneesh Jasuja, Kalpana S. Katti, and Dinesh R. Katti, North Dakota State University, Department of Civil, Construction and Environmental Engineering

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

In this work, we investigated flow structures within the pores of an in-vitro bone model to understand the mechanical micro-environment surrounding cancer cells. The bone scaffold is positioned within the bioreactor under a constant flow rate, delivering the media to the cancer cells. The cells are seeded to grow on the surface of the scaffold for 23 days before being harvested for analysis. Based on the micro-Computed Tomography scans from the in-vitro experiments, we created a full-scale 3D surface mesh of the scaffold using open-source software Slicer3D and Meshmixer. Using the commercial meshing software Gridgen Pointwise we created the computational grid. We performed Computational Fluid Dynamics (CFD) simulations with the immersed boundary method to investigate the flow patterns inside the pores of the scaffolds. We carried the post-pressing of the results with the open-source software ParaView and Blender to create a high-resolution visualization of the flow within the scaffold's complex porous geometry. The flow velocity and the wall shear stress distributions inside the scaffold appear convoluted and highly sensitive to the pore size. The computational results show a distinctive difference in the shear stress distribution on the scaffold's sides. Our results suggest that there is a link between interstitial flow patterns and cancer cell growth.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37296

#18 **Investigation of Blood Flow Dynamics in Intracranial Aneurysms using High-Resolution CFD Simulation**

Tam Thien Nguyen, Davina Kasperski, and Trung Bao Le, North Dakota State University, Department of Civil, Construction and Environmental Engineering

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

We use High-resolution CFD simulation to investigate the dynamics of blood flow in brain aneurysms. We also implement a state-of-the-art code for solving the flow equations. In addition, patient-specific MRA data are processed to generate 3D geometries of aneurysms. The results allow us to investigate the dependence of the degradation of the aneurysm walls

with the flow instabilities. High-resolution CFD simulation is robust for the variety of shapes, sizes, and complexity of intracranial aneurysms.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37400

#19 **Long Term Effect of BMPs on In-Vitro Bone Regeneration using Nanoclay Scaffolds**

Krishna Kundu, Sharad V Jaswandkar, Dinesh R. Katti, and Kalpana S. Katti, North Dakota State University, Department of Civil, Construction and Environmental Engineering

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

The present study focuses on the development of nanoclay based interlocking scaffold and study the long-term effect of the BMPs in bone regeneration. We observed enhanced cell viability, osteogenic differentiation, ECM formation, and improved nanomechanical properties with BMPs coated scaffolds compared with uncoated scaffolds. This study provides valuable insight into the mechanisms of the BMPs through the activation of the Wnt/β-catenin signaling pathway, and enhanced ECM formation leading to higher modulus at extended time periods.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37346

#20 **Modal analysis of blood flow in brain aneurysms**

Davina Kasperski, Lahcen Akerkouch, Trung Bao Le, Sanford Heath, North Dakota State University, Department of Civil, Construction and Environmental Engineering

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

Current risk factor calculators lack necessary data related to intra-aneurysmal blood flow dynamics, (Rayz & Cohen-Gadol, 2020). In this study, we aim to represent the findings in a detailed methodical report describing the features of the flow. The report in turn can help neurosurgeons decide on the best treatment for a specific patient.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37331

#21 **Multifunctional Nanoparticles for Synergistic Photodynamic / Photothermal Therapy**

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

ND-ACES
Sponsors: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202, National Science Foundation grant CHE 1709160, and NIH COBRE grant as Project Director (2P20GM104360-06A1; P.I. R. Vaughan)

The goal of this study was to develop a multifunctional nanoparticle that shows the high therapeutic efficiency of cancer treatment. To achieve this, we used PSMA as a crosslinker and incorporated Mn ions to produce O_2 because of H_2O_2 catalysis to reverse the hypoxic tumor microenvironment and improve the therapeutic efficiency of Photodynamic therapy, PCPDTBT was used as a near-infrared absorption agent and subsequent value in improving Photothermal Therapy efficiency.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37329

#22 **Nanomechanics of Actin Filament Deformation and Fracture: A Steered Molecular Dynamic Study**

Sharad V. Jaswandkar, Kalpana S. Katti, and Dinesh R. Katti, North Dakota State University, Department of Civil, Construction and Environmental Engineering

ND-ACES

Sponsors: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202, NDSU Grand Challenge Center for Engineered Cancer Testbeds. Computationally Assisted Science and Technology (CCAST), NDSU. Materials and Nanotechnology Program, NDSU. Civil and Environmental Engineering Department, NDSU

In the present investigation, steered molecular dynamics (SMD) simulation approach has been utilized to understand the influence of ADF/cofilin binding on actin filament's (F-actin's) deformation and severing mechanics. The work is performed in three computational experiments: tension, compression, and bending. We discovered that structural changes in F-actin induced by ADF/Cofilin play a critical function in regulating its depolymerization and severing. The F-actin mechanics described here are vital for constructing a mechanobiological eukaryotic cell model that mimics cell mechanics with disease progression.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37351

#23 **Photo-induced Charge Transfer of Fullerene and Non-fullerene Conjugated Polymer Blends via *ab initio* Excited-state Dynamics**

Amirhadi Alesadi, Wenjie Xia, and Dmitri Kilin, North Dakota State University, Department of Civil, Construction and Environmental Engineering

ND-ACES

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202, ND EPSCoR through the New Faculty Award, the Department of Civil, Construction and Environmental Engineering, and the College of Engineering at North Dakota State University, the supercomputing resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility located at Lawrence Berkeley National Laboratory, NSF CHE 2004197 for exploration of charge transfer and NSF CHE 1944921 for developing methods of quantum dynamics

Organic conjugated polymers (CPs) are promising candidates for organic photovoltaic (OPV) devices due to their unique tunable mechanical and optoelectronic performance. However, their power conversion efficiency is still lower than their inorganic counterparts (i.e., silicon), limiting their practical usages. In this study, we employ *ab initio* molecular dynamics, to explore photo-induced charge transfer (CT) of diketopyrrolopyrrole (DPP) based polymer as a blend with non-fullerene (i.e., ITIC) and fullerene (i.e., PCBM) acceptor units. Our research aims to explore bulk heterojunctions (BHJ) electronic performance for OPV devices and narrow down the list of potential donor-acceptor candidates.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37247

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

Zachary J. Bailey, Vladimir V. Zotov, and Guodong Du, University of North Dakota, Department of Chemistry

ND-ACES

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

Polymeric nanoparticles present a method for cancer treatment through selective targeting and controlled release of drugs. Poly(silyl ether)s (PSEs) based nanoparticles show promising use due to the presence of an Si-O-C bond exhibiting hydrolytic degradation. 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 release of payload by these nanoparticles are being studied and optimized.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37385

#25 **Polyglutamic Acid, Chitosan and sodium alginate-based calcium assisted hydrogel for cell supporting artificial cell bed**

Raj Shankar Hazra, Md Rakib Hasan Khan, and Mohiuddin Quadir, North Dakota State University, Department of Coatings and Polymeric Materials

ND-ACES

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

Artificial tissue engineering is an emerging field as tissue mimicking artificial cell bed can be huge replacement over current animal-based study. In our study we have selected biobased polymers such as Polyglutamic Acid (PGA), Chitosan (CS) and sodium alginate (SA) and prepared hydrogel with assistance of calcium (Ca2+) ion and used as cell bed for cell support.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37342

#26 **Prostate Cancer Cells Grown on Polyglucuronic Acid Polymer Scaffolds**

Sierra Giebel, Sujata G. Birua, Jackson Haug, and John C. Wilkinson, North Dakota State University, Department of Chemistry and Biochemistry

ND-ACES

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

Approximately 1 out of every 8 men will be diagnosed with prostate cancer within their lifetime. If caught early, prostate cancer has a high 5-year survivability rate. However late-stage prostate cancer metastasizes to bone and results in a grim prognosis. Using polyglucuronic acid polymer scaffolds will allow us to closely mimic the environment of the tumor *in* vivo and will give us a better understanding of late-stage prostate cancer and ultimately how to treat it.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37302

#27 **Rapid Synthesis of N-[1-(4-isopropylphenyl)ethyl]formamide**

Lynn I. Vick, Lioudmila I. Bobyleva, and Mikhail M. Bobylev, Minot State University, Division of Science – Chemistry

ND-ACES

Sponsor: National Science Foundation 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-isopropylphenyl)ethyl]formamide. The reaction was conducted on a 10 mmol scale at 180-189 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 of N-[1-(4-isopropylphenyl)ethyl]formamide was 87.6%.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37727

#28 **Rhodiola crenulata induces apoptosis 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, and Kalpana S. Katti

ND-ACES

Sponsors: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202, NDSU Grand Challenge Center for Engineered Test Beds, ND, APUC 46000ACES-1946202, ND dept. of Agriculture

Advanced stage breast cancer is a fatal disease in which many of the current anti-cancer therapeutics are ineffective due to lack of accurate screening models. Rhodiola crenulata is a Tibetan plant-based extract that is recently shown to be effective for primary site breast cancer. In this study, we tested Rhodiola crenulata on our 3D *in vitro* model of bone

metastatic breast cancer. We have performed various cellular bioassays to elucidate the cytotoxicity of Rhodiola Crenulata.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37353

#29 **Size-Dependent Structural Behaviors of Polymer Tethered, Crumpled Graphene Sheet**

Amara Arshad, Wenjie Xia, North Dakota State University, Department of Civil, Construction and Environmental Engineering
ND-ACES
Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

To understand the dynamics of interfacial structural behavior of complex graphene sheet with tethered polymers at fundamental level is of critical importance in various engineering, health, and technological applications. Here we employ coarse-grained molecular dynamics simulation to model the behavior of PMMA tethered graphene under geometric confinement and elucidate the effect of chain length and grafting density, with a focus on the structure stabilizing mechanisms and symmetry properties of the crumpled sheet. The simulation results reveal that tethered graphene sheets with increase chain length and grafting density of 0.3 chains/nm^2 at the initial two-dimension (2D) state tends to become more self-adhering and self-folding upon crumpling compared to the smaller ones, before forming a sphere-like highly crumpled structure. Remarkably, by evaluating the shape descriptors, it is found that the crumpling behaviors of tethered graphene sheet is associated with edge bending and self-folding. These findings provide fundamental insight towards the feasibility of using crumpled graphene in place of pristine graphene in applications involving crumpled carbon structures.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37307

#30 ***Streamlined Synthesis of Dual-Emissive Fluorescent Silicon Quantum Dots (SiQDs) for Cell Imaging***

Di Sun, Xu Wu, Jeremy Martin, Kirati Tayutivutikul, Diane Darland, and Julia Xiaojun Zhao, University of North Dakota, Department of Chemistry
ND-ACES
Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202, NSF grant CHE 1709160, NIH COBRE grant as Project Director (2P20GM104360-06A1; P.I. R. Vaughan

We have developed a one-pot synthetic route to produce a dual-emissive silicon quantum dots (SiQDs) using a hydrothermal method. The obtained SiQDs showed an average size of 4.9 ± 0.2 nm with two fluorescence emission peaks (450 nm, 836 nm) under one excitation wavelength of 357 nm. The SiQDs were characterized using UV−vis absorption spectroscopy, fluorescence spectroscopy, dynamic light scattering (DLS), Fourier transform infrared spectroscopy (FTIR), high-resolution transmission electron spectroscopy (HRTEM), and X-ray photoelectron spectroscopy (XPS). The effect of SiQDs on cell viability was evaluated using brain-derived microvascular endothelial cells (MVEC), neural stem cells (NSC) and fibroblast cells (MVFB) under different concentrations of SiQDs. Finally, the SiQDs was successfully applied to in vitro fluorescence imaging with several cells, including neural stem cells (NSC), brain-derived microvascular endothelial cells (MVEC), and brain-derived microvascular fibroblast cells (MVFB), and SiQDs were provided a robust signal localized primarily around the nucleus and throughout the cytoplasm. The results demonstrated that SiQDs would be promising fluorescence labeling materials for imaging a wide variety of cells.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37316

#31 **Synergistic Anticancer Effects of All-Trans Retinoic Acid and Doxorubicin**

Connor Edvall (NDSU), Nicholas Bittner (CCCC), Brent Voels (CCCC), Michael Parker (CCCC), and Sanku Mallik (NDSU), North Dakota State University,

Department of Pharmaceutical Sciences, Cankdeska Cikana Community College and Turtle Mountain Community College
ND-ACES
Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202
Hypoxia is a state of the tumor microenvironment in which oxygen levels are low in the tumor. This can lead to increased metastatic activity along with increased resistance to anticancer drugs. Thus, alternate methods are required to treat tumors that have become hypoxic. The methods we will be using are nanocarriers in the form of hypoxia responsive polymersomes to penetrate the tumor and synergistic treatment with the encapsulated anticancer drugs Doxorubicin and All-Trans Retinoic Acid.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37330

#32 **Synthesis and Characterization of Degradable Hyperbranched Poly(silyl ether)**
Vladimir Zotov, Zachary Bailey, and Guodong Du, University of North Dakota, Department of Chemistry
ND-ACES
Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202
Hyperbranched polymers give rise to different properties than linear polymers such as high surface areas and open ending groups allowing further functionalization. Poly(silyl ether)s (PSEs) have good degradation properties which can be used in several applications in industrial, environmental, and medicinal fields. In this study, hyperbranched PSEs have been synthesized by an $A_2 + B_3$ approach and their properties are being fully characterized, particularly for medicinal applications.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37306

#33 **Synthesis of N-[1-(4-hydroxyphenyl)ethyl]formamide**
Hassan Elshanbary, Lioudmila I. Bobyleva, and Mikhail M. Bobylev, Minot State University, Division of Science – Chemistry
ND-ACES
Sponsor: National Science Foundation 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-hydroxyphenyl)ethyl]formamide. The reaction was conducted on 10 mmol scale at 180-200 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 15 minutes. The isolated yield of N-[1-(4-hydroxyphenyl)ethyl]formamide was 82.2%.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37729

#34 **Synthesis of red-emissive porphyrin-based graphene quantum dots (PGQDs) using biomass-derived material for *in vitro* cell imaging**
Sarah Reagen, Yingfen Wu, Rahul Shahni, Wen Sun, Jin Zhang, Qianli R. Chu, Xiaodong Hou, Colin Combs, and Julia Xiaojun Zhao, University of North Dakota, Department of Chemistry
ND-ACES
Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202, NSF grant CHE 1709160, and we would like to formally thank Henrietta Lacks and her family for the contribution of HeLa cells
Red and near infrared emission light is a highly desirable feature for fluorescent nanoparticles in biological applications mainly due to longer wavelengths more easily being able to penetrate tissues, organs, skin, and other organic components. In this work, meso-tetra(4-carboxyphenyl)porphine (TCPP) is used in tangent with *cis*-cyclobutane-1,2-

dicarboxylic acid (CBDA-2), a biomass derived organic molecule, to synthesize “green” porphyrin-based graphene quantum dots (PGQDs) with red-emission light and improved photostability for *in vitro* confocal cell imaging.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37313

#35 **System for Image Segmentation on Supercomputers**

Zakaria El Mrabet, Traver Bradley, David Apostal, and Aaron Bergstrom, University of North Dakota, Computational Research Center
ND-ACES
Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

The purpose of this study is to implement a system for image segmentation on supercomputers. It consists of different components, including Singularity, CUDA, and Caffe U-Net. It would assist researchers in running image segmentation in various applications such as biometrics, medical image analysis, and crop disease detection.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37299

#36 **The Mechanical Response of Force Activated Integrin using Molecular Dynamics**

Hanmant Gaikwad, Sharad Jaswandkar, Kalpana S. Katti, and Dinesh R. Katti, North Dakota State University, Department of Civil, Construction and Environmental Engineering
ND-ACES
Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202, the NDSU Grand Challenge funded Center for Engineered Cancer Testbeds, and the support of the computational resources at NDSU CCAST

The integrin is the cell surface protein, couples the extracellular matrix (ECM) to the cell cytoskeleton, and facilitates cell migration, proliferation, and differentiation. Its role as a mechanotransducer and signaling molecule implicates the cancer progression from the primary tumor to metastasis. Furthermore, it acknowledged the importance of integrin in transmitting and sensing mechanical force. Therefore, this study aims to predict the mechanical properties of integrin for integrin-based adhesion by using steered molecular dynamics (SMD).
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37325

#37 **Thermomechanical and Dynamics Properties of Polymer – Clay Nanocomposites**

Wenjian Nie, Yangchao Liao, Zhaofan Li, and Wenjie Xia, North Dakota State University, Department of Civil, Construction and Environmental Engineering
ND-ACES
Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

Polymer - clay nanocomposites (PCNs) are commonly applied as multi-functional structural materials with superior thermomechanical and dynamics properties while maintaining the characteristics of lightweight and optical clarity. As a result, adding of nanoclays can significantly affect the thermomechanical and dynamic properties of polymers such as mean-square displacement, molecular stiffness, Young’s modulus and shear modulus, which remains to be better understood. To this end, We implement the coarse-grained (CG) dynamics simulation to investigate PCNs properties.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37317

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

Anupom Deb Nath, Stefan W. Vetter, North Dakota State University, Department of Pharmaceutical Sciences
ND-ACES

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

The extracellular matrix (ECM) is an important component of solid tumors and, developing models of the ECM of cancer patients could be an important contribution to develop novel cancer therapeutics. Our project investigates the consequences of artificial aging of ECM on cancer cell behavior and the differential regulation of genes involved in cancer cell invasiveness. The studies are being performed using 2D- and 3D-cell culture support beds. Initial study results will be presented.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37338

#39 **Transfer Learning Pre-training Dataset Effect Analysis for Breast Cancer Imaging**

Chanaka Bulathsinghalage, Lu Liu, North Dakota State University, Department of Computer Science
ND-ACES
Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

Comparing with natural imaging datasets, the effects of medical pre-training datasets are underexplored. We carry out transfer learning pre-training dataset effect analysis in breast cancer imaging by evaluating neural networks on target datasets under fine-tuning configurations. The pre-training dataset, DDSM, is effective on the mammogram datasets and ineffective on the ultrasound dataset. Also, fine-tuning may mask the inefficacy of a pre-training dataset. In addition, representational analysis and hybrid transfer learning performance evaluation are carried out.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37290

#40 **Transfer Learning Pre-training Dataset Effect Analysis for Histopathology Cancer Images**

Koushik Howlader, North Dakota State University, Department of Computer Science
ND-ACES
Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

The existing pre-training image classification models are more efficient for natural images in comparison to medical imaging, particularly histopathology images. In this experiment, we demonstrated the ability of transfer learning pre-training dataset for histopathology cancer images by considering three deep neural networks VGG16, ResNet50, and InceptionV3 on four other types of cancer histopathology image target datasets. Finally, it can be concluded that performances are much improved while objective datasets are tested with the pre-trained model.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37327

#41 **Understanding the Impact of Covid-19 on Online Cancer Support Community**

Md Al-Amin, Lu Liu, North Dakota State University, Department of Computer Science
ND-ACES
Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202

Similar previous pandemic, COVID-19 pandemic has an immense implication on health challenges. We study to better understand the impact of COVID-19 pandemic on cancer patients through examining discussions within cancer support communities on Reddit. First, determine the rate of submissions and comments before and after pandemic to understand the influence of COVID-19. Next, analyze text data, implement LDA topic modeling to extract hidden information. Finally, build user-interaction graphs to understand users' behavior in the community.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37309

#42 **Understanding The Properties of Non-Natural Amino Acids for Clay-Material Binding**

Sean Glaholt, Atir Kaunain, and Mark Hoffmann, University of North Dakota, Department of Chemistry

ND-ACES

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1946202, also acknowledged: Tao Yu (Deceased) and Jabed Mohammed

In this study, we employed the density functional theory method to investigate structures and properties on six non-natural amino acids (NAA). Using *Gaussian09* and *Avogadro*, we first optimized the geometries of the target NAA in both the gas phase and aqueous solution phase with the PCM model. The atomic charges in each NAA were calculated, and this information will be useful to understanding the interactions between NAA and clay materials. Meanwhile, the HOMO/LUMO orbital, and the electrostatic potential information of each NAA were investigated.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37320

#43 **Machine Learning multimodal analysis of cell-free DNA sequencing for cancer detection and tissue of origin localization**

Nazim Belabbaci, University of North Dakota, Department of Biomedical Engineering

ND-ACES

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

Cell-free DNA (cfDNA) has been instrumental in today's research about cancer detection and diagnosis. People with infectious diseases may have tumors in their blood with genetic markers different from the normal (healthy) cells and specific to the tumor. DNA sequencing allows us to uncover those markers and look for mistakes that may be driving the disease. Artificial intelligence (AI) and machine learning (ML) are speeding up that process and making it more efficient and accurate by sifting through all the data and finding patterns the human eye can't see. In this study, we perform a comparative analysis of well-known ML techniques, including Linear support vector machines, feed-forward neural networks, random forest, and binomial generalized linear models with elastic-net regularization for a prediction model for cancer detection. The goal of this research will be to come up with the most efficient DNA sequencing classifiers first for cancer detection, then a prediction model for the tissue of origin localization.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37334

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

Carson Herbert, Jarret Merschman, Motoki Takaku, and Archana Dhasarathy, University of North Dakota, Department of Biomedical Sciences

ND-ACES

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

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.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37288

#45 **The Effects of Arabinoxylan on Gut Flora Immunity**

Taylor Stegman, Brooke Roeges, Hayle Boechler, Khwaja Hossain, and Michael Kjelland, Mayville State University, Division of Science & Mathematics

ND-ACES

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 growth and development of beneficial gut bacteria.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37352

3D Culture Model to Mimic the Heterogeneity of Breast Cancer

Sujata Birua, Sierra M. Giebel, Annie J. Schiro, and John C. Wilkinson, North Dakota State University, Department of Chemistry and Biochemistry

ND-ACES

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

Roughly 90% of potential anti-cancer drugs fail in part due to incomplete preclinical models that poorly represent the *in-vivo* tumor microenvironment. Animal models are valuable but expensive and time-consuming, and two-dimensional culture system lacks the heterogeneity and physiology of tumor environment. Therefore, the present study aims to optimize the novel, next-generation scaffold formulations based on chitosan polymers that can serve as three-dimensional culture systems for heterogeneous breast cancer tissue growth and subsequent drug testing trials.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37295

Developing and Refining Tasks for ND-ACES Bioscience Modules

Ryan Summers, Jill Baird, Sarah Boese-Noreen, Laurie Kok, University of North Dakota, Department of Teaching, Leadership, and Professional Practice

ND-ACES

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

During ND-ACES Year 2, Education and Workforce Development faculty and research assistants have planned and assembled a bioscience module. All instructional materials and tasks included in the module have been selected to support middle and high school teachers and students. The poster will detail how the contents of the bioscience module creates opportunities to connect research topics to the required content and performance expectations at these levels.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37356

Engineering

A Review of Fate and Transport of Microplastics in the Natural Environment

Mansurat Abdulmalik Ali and Xiao Feng, University of North Dakota, Department of Environmental Engineering

Engineering, Life Sciences, STEM Education and Learning Research

Sponsor: The National Science Foundation under NSF EPSCoR, the NDWRRI Fellowship grant awarded from the USGS annual 104b base grant and the ND SWC fund

Microplastics are emerging persistent environmental pollutant of increasing concern with major pathways either by land or water through which they are disposed/transported and making them a point of contact for microplastic pollution and possibly, a pathway into the food chain. Although microplastics have been extensively detected in the natural environments (soil and water) using methods of identification and characterization such as SEM, TGA, FT-IR and Raman Spectroscopy, these methods are not consistent in data computation, they are inefficient, time consuming and labor intensive and there is no standardized method available for quantification. This research is designed to explore, a fast, consistent, reliable, and efficient method of microplastic identification in the natural environment.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37469

A Unique Fast-Charging Technique for Li-ion Batteries in Cold Temperatures

Shabaz Khan, Michael Mann, Xiaodong Hou, and Daniel Laudal, University of North Dakota, Institute for Energy Studies, College of Engineering and Mines

Engineering

Sponsor: Research presented in this poster was supported by ND EPSCoR

Range anxiety and recharging time are two biggest obstacles for Electric Vehicle (EV) growth. Our proposed unique hybrid fast charging technique is operational in cold temperature. The goals of this work are: 1) charge a battery to 90% within 15 minutes, 2) keep battery cycle life longer, and 3) keep electrode chemistry independent. The technique internally pre-heats the battery before fast charging to lower heat loss without sacrificing cycle life while maximizing the benefits.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37336

Context-awareness for close-proximity human-robot collaboration during construction tasks

Sajib Sarkar, Youjin Jang, and Inbae Jeong, North Dakota State University, Department of Civil, Construction and Environmental Engineering

Engineering

Sponsor: The ND EPSCoR STEM grants program

This study proposes a novel method for 3D human pose estimation. 2D joint locations were extracted from images captured by multi-camera, and the 3D human pose was then approximated using the particle filtering technique to fuse 2D joint locations probabilistically. The proposed method was evaluated in both simulation and laboratory settings, and the results demonstrated the accuracy of estimation and the feasibility in practice. This study contributes to ensuring human safety in close-proximity human-robot collaboration.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37285

Decomposition of perfluoroalkyl and polyfluoroalkyl substances (PFASs) in chlorinated drinking water

Runze Sun and Feng Xiao, University of North Dakota, Department of Civil Engineering

Engineering

Sponsor: Early Career Award from the U.S. Environmental Protection Agency Science to Achieve Results (STAR) Program, Department of Defense, and the U.S.

National Science Foundation CAREER Program. YB was supported by the University of North Dakota Pilot Postdoctoral Program from the Office of Vice President for Research & Economic Development

Chlorination is the most widely used technique for disinfection of drinking water. The disinfection by-products (DBPs) resulting from the reaction of chlorine with per- and polyfluoroalkyl substances (PFAS) are not clear. The study investigated decomposition of PFAS during chlorination of synthetic water and natural surface water. The results demonstrated generation of certain PFASs from precursors during chlorination. Identification and semi-quantitative yields of DBPs also revealed different fates of PFASs depending on their structures.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37321

First Comprehensive Investigation of Volatiles Generated from PFAS-containing Aqueous Film-forming Foams and Commercial Fluorosurfactants in Pyrolytic Processes

Bin Yao, Alena Kubátová, and Feng Xiao, University and North Dakota, Departments of Civil Engineering and Chemistry

Engineering

Sponsor: ND EPSCoR and UND postdoctoral award

This study reveals the *de novo* formation of 1,4-dioxane, heteroaromatics, and aromatics (e.g., benzene and styrene) during PFAS-containing aqueous film-forming foam (AFFF) and commercial surfactant concentrates (SC) thermal treatment. 1,4-Dioxane and aromatics were found as main toxic pyrolyzates at 300–890 ^{o}C, likely formed as a consequence of dehydration, dehydrogenation, and cyclization of glycols and glycol ethers detected in AFFFs and SCs. Octylphenol and octylphenol polyethoxylate were found in AFFFs but not in SCs.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37303

Immunofluorescent staining of pathology images using a machine learning approach: A tumor microenvironment study in Breast Cancer

Benu Bansal and Sandeep Singhal, University of North Dakota, Departments of Biomedical Engineering and Pathology, School of Medicine and Health Sciences, School of Electrical Engineering and Computer Science

Engineering

Sponsor: The National Institute of General Medical Sciences of the National Institutes of Health under Award Number U54GM128729

The tumor microenvironment (TME) has broadly implied the existence of carcinogenesis. It accommodates tumor cells that interact with surrounding cells through the circulatory and lymphatic systems to influence cancer development. The TME gives cancer all of the nutrients it needs and makes space for cancer to expand. This research aims to apply image analysis to examine the tumor microenvironment and offer deeper insight into our understanding of the tumor to the microenvironment.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37339

Impact of Indoor Environmental Quality on School Children: Monitoring and Assessment

Xiaoou Hu and Yao Yu, North Dakota State University, Department of Civil, Construction and Environmental Engineering

Engineering

Sponsor: ND EPSCoR STEM grants program

Indoor Environmental Quality (IEQ) plays a significant role in affecting people's comfort, health, and cognitive function, especially for children. This project aims to collect community-based data through a literature review and a survey for the future NSF grant application, where the research team will develop a protocol allowing real-time, long-term monitoring and

assessment of critical IEQ parameters to establish a community-level IEQ evaluation of homes and schools for elementary school children.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37280

Insulation Performance of Silica Aerogel Blanket for Protecting Advanced Performance Monitoring systems used in Space Applications under Extreme Temperature Environments

Ratna Yasoda and Ying Huang, North Dakota State University, Department of Civil, Construction and Environmental Engineering

Engineering

Sponsor: The National Aeronautics and Space Administration under NASA EPSCoR Cooperative Agreement Notice (CAN) award # FAR0031089

The present work investigated the insulation protection performance of different thicknesses of silica aerogel blankets (SAB) in protecting the performance monitoring systems such as sensors (operating temperatures are under 120°C) used in spacecraft when ambient temperatures are 460°C. The results of the study indicated that a 15 mm thick SAB provides required insulation, and proved to guard the Fiber Bragg Grating (FBG) sensors when the ambient temperature is maintained at ~ 460°C
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37355

Luminal Master Regulator Gene Expression in Patients with Breast Cancer

Kalli Schaefer and Sandeep Singhal, University of North Dakota, Departments of Biomedical Engineering and Pathology, School of Medicine and Health Sciences, School of Electrical Engineering and Computer Science

Engineering

Sponsor: The National Institute of General Medical Sciences of the National Institutes of Health under Award Number U54GM128729.

Accounting for 12% of breast cancers in the United States between 2012 and 2016, triple-negative breast cancer has a poor prognosis when compared with other subtypes of breast cancer and women of African heritage tend to suffer from triple-negative breast cancer more frequently. This study found that luminal master regulator genes ESR1, FOXA1, and GATA3 were useful in predicting breast cancer survival based on race.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37349

Soybean Cyst Nematode Detection and Management using Multispectral Imaging and Machine Learning.

Niroop Sugunaraj (UND), Youness Arjoune (UND), Sai Peri (UND), Sreejith V. Nair (UND), Anton Skurdal (UND), Jaya Preethi Mohan (UND), Prakash Ranganthan (UND), and Burton Johnson (NDSU), University of North Dakota Department of Electrical Engineering and North Dakota State University Department of Plant Sciences

Engineering

Sponsor: The National Science Foundation under NSF EPSCoR #UND0026828 and by the North Dakota Agricultural Products Utilization Commission (APUC) under #UND0025510

Soybean yields suffer significant losses every year due to a plant parasite called soybean cyst nematode (SCN). To overcome the challenges of manual soil sampling to detect SCN, deep learning and multispectral imaging are
important in precision agriculture to detect disease due to SCN. Recommendations for soybean research using deep learning and multispectral imaging for sufficient training and testing methodologies are essential for deeper analyses.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37289

Spatial Frequency Domain Imaging

Kristen Stromsodt and Bo Liang, University of North Dakota, Department of Biomedical Engineering, School of Electrical Engineering and Computer Science, College of Engineering and Mines

Engineering

Sponsor: None

Human tissue is made of numerous chemical constituents. These help reveal the state of disease in a sample. Optical imaging can measure these properties non-invasively. In this study, we describe a portable spatial frequency domain imaging system. The system works by projecting sinusoidal light patterns onto a sample, processing the reflectance, and determining properties of the tissue. We can use the properties of the sample to help physicians make a diagnosis in real time.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37328

Chemistry

Carbon-Carbon Bond Formation Using Cyclopalladated Complexes and Boronic Acids

Purna Chandra Rao Vasireddy and Irina P. Smoliakova, University of North Dakota, Department of Chemistry

Chemistry

Sponsor: The University of North Dakota

We report a new approach to the formation of (sp^2)C–(sp^2)C, (sp^2)C–(sp^3)C, and (sp^3)C–(sp^3)C bonds using reactions of [(sp^2)*C,N*]- and [(sp^2)*C,N*]-cyclopalladated complexes (CPCs) with arylboronic acids. The scope of CPCs and boronic acids, which can be used for this transformation, was determined, and the reaction conditions, i.e., temperature, base and solvent, were optimized. The product yields were in a range of 10-90%. The stereoselectivity of this transformation was studied using two diastereomeric CPCs with a chiral center directly bonded to the metal. Compounds isolated in this study were characterized by ^{1}H, ^{13}C, NOESY, COSY and HSQC NMR spectra and HRMS data. X-ray crystallographic data of a chiral product is also reported.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37911

Metal Oxide Nanoparticles at Functionalized Graphene Surface for Electrochemical Supercapacitors

Wen Sun, David Pierce, and Julia Xiaojun Zhao, University of North Dakota, Department of Chemistry

Chemistry, Materials Research

Sponsor: The National Science Foundation Award Number CHE 1709160

In developing alternative renewable and sustainable energy supplies, supercapacitors, have attracted notable attention due to environmental friendliness, the capacity of safely providing high power, rapid charging with extremely long cycle life, lightweight, and flexible portable devices properties. The materials of electrodes are essential parts of a supercapacitor, particularly their conductivities and activity surface areas. The current method is based on the reduction of metal precursors and graphene oxide (GO) in a single step using glucose as a reducing agent. The rGO is a substrate for the homogeneous growth of metal oxide nanoparticles to improve the electrical conductivity, while the metal oxide nanoparticles can serve as a separator to inhibit the aggregation of the rGO and maximize the specific capacitance. The proposed synthetic method is accomplished without any annealing or calcination process. This is an advantage in reducing energy consumption during the preparation step.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37322

Near-Infrared Studies of Cu (I) Dipyrrin Complexes: Effect of Conjugation and Substituting groups

Omolola Eniodunmo and Svetlana Kilina, North Dakota State University, Department of Chemistry and Biochemistry

Chemistry

Sponsor: The DOE Grant DE-SC0022239. This work used resources of the Center for Computationally Assisted Science and Technology (CCAST) at North Dakota State University, which was made possible in part by NSF MRI Award No. 2019077.

This work investigates the photo-physical properties of Cu (I) Dipyrrin complexes in the near infrared region via structure modification for application in biomedical fields such as photodynamic therapy. We use time-dependent density functional theory to study the optical properties of these complexes and employ Redfield master equation dynamics to explore photoluminescence quantum yield. Our calculations suggest that modifying conjugation and electronegativity of the substituent group shows tunable optical features for direct use in many applications.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37297

Novel Sensor Materials for In-situ Resource Utilization in NASA Explorations – Adsorption of Small Molecules on Graphene and Pt/Graphene

Uwe Burghaus and Thomas Stach, North Dakota State University, Department of Chemistry and Biochemistry

Chemistry

Sponsor: 2022 ND NASA EPSCoR Supplemental Project Funding Award

The object is the characterization (sensitivity/reactivity, selectivity) of novel materials relevant for the next generation of gas sensors used in NASA missions. According to thermal desorption spectroscopy (a kinetics techniques) and Auger electron spectroscopy, H_2S and SO_2 dissociate on graphene, epitaxially grown on Ru(0001) with a reaction probability of 50%. O_2, SO, and H_2 desorb, sulfur remains on the surface. Studying CO, CO_2, and H_2 adsorption on Pt clusters, deposited on graphene is in progress.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/36697

Photoluminescence of Cis- Polyacetylene Semiconductor Material

Kamrun Nahar Keya, Mohammed Jabed, Wenjie Xia, and Dmitri Kilin, North Dakota State University, Department of Civil, Construction and Environmental Engineering

Chemistry, Engineering, Materials Research

Sponsors: NSF CHE-1944921 for development of methods for excited state dynamics and DOE DE-SC0021287 for research of one-dimensional infrared emissive materials. National Energy Research Scientific Computing Center (NERSC) and North Dakota Established Program to Stimulate Competitive Research (ND EPSCoR) and CCAST Thunder Cluster at NDSU.

Photoluminescence (PL) is an important characterization technique used to characterize optoelectronic materials, including conjugated polymers. To explain PL [1] cis-polyacetylene oligomer is used. In this study, we investigate the coupling between electronic and vibrational properties during photoinduced processes in a specific material. The main result of this research is computational proof of high-intensity inter-band and intra-band optical transitions contributing to photoluminescence spectral signatures of polyacetylene using Redfield equation of motion [2-4].

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37294

Synthesis and Properties of Cyclobutane-containing Anhydrides

Houssein Amjaour and Qianli R. Chu, University of North Dakota, Department of Chemistry

Chemistry

Sponsors: NSF EPSCoR Award OIA #1355466, Members in Chu group, and UND Chemistry Department

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 a 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 the fusion of cyclobutane to the cyclic anhydride functional group.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37514

The Analysis of Photophysical Properties of Organic Complexes Influenced by Metals, Ligand π-Conjugation and Electron Donating/Withdrawing Groups

Haley Woods, Wenfang Sun, and Svetlana Kilina, North Dakota State University, Department of Chemistry and Biochemistry

Chemistry

Sponsors: The NSF grant (CHE-1800476). We thank Xinyang Sun, Omolola Eniodunmo, and Dmitri Kilin for fruitful discussions. This work used resources of the

Center for Computationally Assisted Science and Technology (CCAST) at NDSU, which were made possible in part by NSF MRI Award No. 2019077

Photodynamic therapy (PDT) is a promising tool for the treatment and diagnosis of various cancers. To establish the relationship between photophysical properties and molecular structures that enables a systematic design procedure for novel PDT compounds with improved PDT performances, time-dependent density functional theory calculations are performed on several molecular candidates. Our calculations predict that Os(II) complexes with NH_2 substituents are likely to provide better molecular candidates for treatment of a broader scope of cancer types.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37291

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

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

Chemistry

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

Aliphatic polyesters with high glass transition temperature (Tg) are possible by incorporating rigid or bulky moieties and by introducing substituents along or near the polymer backbone. Here we report a series of new polyesters with high Tg (up to 165 oC) via zinc-catalyzed ring-opening copolymerization of epoxides and novel cyclobutane-derived anhydrides. The polymers properties were characterized by NMR, GPC, TGA, and DSC.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/38120

STEM Education and Learning Research

Development and Evaluation of the Assessment of Student Knowledge of Green Chemistry Principles (ASK-GCP)

Krystal Grieger, Annie Schiro, and Alexey Leontyev, North Dakota State University, Department of Chemistry and Biochemistry

STEM Education and Learning Research

Sponsors: NSF DUE#1852045, DUE#2021285, CHE#2050802, and NDSU's NDUS ECOR Award FAR0035075

As implementation of green chemistry into curriculum increases, it is vital that educators have a tool to rapidly measure student knowledge of green chemistry principles. In this poster, we report the development and evaluation of the Assessment of Student Knowledge of Green Chemistry Principles (ASK-GCP). This instrument was shown to be an efficient and accurate instrument to measure student knowledge of green chemistry principles.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37267

Factors Influencing the Formation of Harmful Algal Blooms (HABs) - Review

Meera Gopinath Sujatha, Devarshi Patel, Prakash Ranganathan, and Scott Korom, University of North Dakota, School of Electrical Engineering & Computer Science, College of Engineering & Mines

STEM Education and Learning Research

Sponsor: ND EPSCoR under UND0026820

One of the important environmental hazards faced globally is the presence of Harmful Algal Blooms (HABs) in most water bodies, which create major socio-economic impacts globally. It is estimated that around 45% of the economic impact due to HAB is in public health across the United States. Many factors contribute to the formation of HABs and hence it is essential to study various detection mechanisms related to these factors influencing HABs.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37310

Interpretable Machine Learning for the Planning and Management of Civil Infrastructure Construction Projects

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

STEM Education and Learning Research

Sponsor: ND EPSCoR STEM grants program

Construction is one of the largest sectors in the world economy. Yet, it has a long record of poor performance. Numerous studies have applied machine learning to construction project planning and management to enhance project performances. However, the developed models are rarely adopted by practitioners due to their black-box features. For critical or high-risk decisions, model interpretability is crucial. This study proposes a framework for applying interpretable machine learning to construction project planning and management.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37301

ND EPSCoR STEM Award: Educating Middle School Students about Clinical Trials and Randomized Control Experiments

Ryan Summers, Tanis Walch, Allison Kelliher, Julie Robinson, Arun Bhatta, Marc Basson, Donald Warne, and Rachel Navarro, University of North Dakota, Departments of Teaching, Leadership, & Professional Practice; Public Health, Education, Health & Behavior Sciences; Family Medicine & Community Medicine and Population Health; Counseling Psychology, Education, Health & Behavior Sciences; and UND School of Medicine and Health Sciences (SMHS)

STEM Education and Learning Research

Sponsor: ND EPSCoR through the STEM grants program

We are supporting STEM education and working collaboratively with middle school teachers to plan for meaningful and innovative science education. Data that will be collected in this

project will strengthen external grant submissions, increasing the competitive advantage in North Dakota. This coincides with the ND Science and Technology Plan (2018) to support the development of a biomedical research corridor in the Red River Valley.
https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37360

Computer and Information Science and Engineering

Evaluation of the critical factors and a future towards Machine Learning assisted membrane fabrication

Musabbir Jahan Talukder and Ali Alshami, University of North Dakota, College of Engineering & Mines

Computer and Information Science and Engineering, Engineering, Materials Research

Sponsor: none

Membrane fabrication is a multivariate operation. For a green and cost-effective separation process, transition into the membrane separation is crucial. For that, an efficient method for membrane material selection and optimization of fabrication is needed. Polymer is a potential membrane material with its tunable and wide range of properties. The large enough dataset in explored polymer membranes creates an opportunity for machine learning (ML) algorithms to be explored and gain an understanding of membrane designing for finding desirable separation performance. In this report, we try to stipulate recent efforts to utilize ML to get insights on novel membrane material discovery and fabrication. A future direction in material selection and optimization for membrane fabrication is outlined. In data mining, systematic inclusion of post-fabrication data is discussed. For a better understanding of the fundamental domain knowledge and experimental experience relation, hybrid models are also discussed under the future scope

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37344

GPS/ADS-B Dropout & Erroneous Data - Methods for Detection and Mitigation

Anton Skurdal, Niroop Sugunaraj, Zakaria El Mrabet, Jaya Preethi Mohan, and Prakash Ranganathan, University of North Dakota, School of Electrical Engineering and Computer Science

Computer and Information Science and Engineering

Sponsor: #UND 0026829

Missing or invalid Global Positioning Systems (GPS) and Automatic Dependent Surveillance-Broadcast (ADS-B) data can be a safety and security risk for Unmanned Aircraft Systems (UAS) navigation and Detect and Avoid (DAA) operations. Erroneous, spoofed, jammed, or dropouts of GPS data can result in UAS position, navigation, and timing (PNT) to be incorrect. Dropouts can cause UAS to be unable to detect and avoid other aircraft or cause avoidance of aircraft that do not exist.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37266

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

Computer and Information Science and Engineering

Sponsor: The National Science Foundation (NSF) under NSF CMMI Award No.2113558. The authors also acknowledge the support from the North Dakota Established Program to Stimulate Competitive Research (ND EPSCoR) through the New Faculty Award. This work used supercomputing resources of the CCAST at NDSU, which were made possible in part by NSF MRI Award No. 2019077

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.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37347

Role of Racial Disparity in Clinical Setting: An Ancestry Estimation using Deep Learning

Jappreet Gill and Sandeep Singhal, University of North Dakota, Departments of Biomedical Engineering and Pathology

Computer and Information Science and Engineering

Sponsor: The National Institute of General Medical Sciences of the National Institutes of Health under Award Number U54GM128729

Admixed population arises when two historically separate populations get mixed due to mating. Over the past decade studies of ancestry, estimation has gained a lot of interest due to its use in both population genetics and medicine. The main goal of ancestry estimation is to infer the constitution of an individual's population of origin based on our understanding of natural populations. Self-reported ancestry information has proven to be inaccurate. The use of genetic information can be helpful to accurately measure an individual's ancestral constitution.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37348

In Silico Prediction of the Toxicity of Nitroaromatic Compounds: Application of Super Learner QSAR Approach

Amirreza Daghighi and Bakhtiyor Rasulev, North Dakota State University, Department of Coatings and Polymeric Materials

Computer and Information Science and Engineering

Sponsor: National Science Foundation EPSCoR Track-1 Cooperative Agreement OIA-1355466 and by the State of North Dakota. A.D. also thanks Biomedical Engineering Program for the financial support in form of GRA funding, as well as partial support from DOE DE-SC0021287 grant

Nitroaromatic compounds (NACs) have attracted a lot of attention because of their wide applications in industrial activities, agricultural practices, and domestic products However, they are proved to have environmental toxic properties. Since assessing the toxicity value of NACs is expensive and time consuming, the goal of this study is to utilize machine learning methods to build a quantitative structure-activity relationship (QSAR) model that predicts the toxicity of NACs in vivo.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/38203

Life Sciences

Gene Expression analysis of Arsenic Level in human, and risk prediction of Vitro Carcinogenic Bladder Tumor

Sonalika Singhal, Nathan A. Ruprecht, Donald Sens, Kouhyar Tavakolian, and Sandeep K Singhal

Life Sciences

Sponsor: The ND INBRE IDeA program P20 GM103442 from the National Institute of General Medical Sciences and IDeA DaCCoTA CTR program, U54GM128729, from NIGMS, NIH

The study identified human genes associated with arsenic exposure and linked to molecular mechanisms of cancer. We developed bladder cancer risk predictive models to forecast the outcomes of arsenic exposed in humans. The model shows the highest prediction ability for recurrent bladder tumors based on 3 genes resulting with AUC of 0.94 and 0.75 on training and validation data.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37318

Mathematical Sciences

SIR Model of COVID-19 in North Dakota

Hoang Long Nguyen and Bishnu Sedai, Minot State University, Department of Mathematics and Computer Science

Mathematical Sciences

Sponsor: ND EPSCoR STEM

The SIR model is a famous mathematical model for the study of infectious diseases dynamics. In this research, we study the basic SIR model of COVID-19 in North Dakota. We derive mathematical formulas to estimate its parameters. We modify the model by adding the vaccinated compartment and compute the reproduction number. We study the local stability of the disease-free equilibrium in terms of basic reproduction number in both vaccinated and unvaccinated cases.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37300

Time Series Analysis in Forecasting Average Monthly Rainfall and Temperature

Upul Rupassara, Favour Ozordi, and Dion Udokop, Minot State University

Mathematical Sciences

Sponsor: ND EPSCoR

This project analyzes the monthly average rainfall and temperature data from 2005 January to 2021 December in Minot ND. Graphical analysis with ACF, PACF plots, and AIC, BIC criteria were used to find the best fitting model that capture the pattern of the data set. Also, diagnostic and residual analysis techniques were used to further analyze the fitted models. Among the competitive models, SARIMA (2,0, 2) (0, 1, 1, 12) and SARIMA (1, 1, 1) (2, 0, 2, 12) are found to be the best models that can be used to forecast the average rainfall and temperature data respectively.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37274

Materials Research

Understanding the size effects on the crumpling behaviors of nanoribbons

Yangchao Liao, Oriana Molares Palmero, Zhaofan Li, Wenjian Nie, and Wenjie Xia, North Dakota State University, Department of Civil, Construction and Environmental Engineering

Materials Research

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Understanding the complex crumpling behaviors of nanoribbons at a molecular level is of critical importance in various engineering and technological applications. Here, we report the results of a systematic coarse-grained molecular dynamics (CG-MD) simulation study of the crumpling process of nanoribbons at various aspect ratios in the case of graphene. By evaluating the evolution of potential energy of the nanoribbon during the crumpling process, our results show that the increase of the aspect ratio greatly enhances the adhering effect of the nanoribbons to form a scroll configuration in quasi-equilibrium. Moreover, two aspect ratio dependent crumpling modes were found, which are the random bending and folding dominated crumpling mode, and the bending, sliding and folding along the length direction dominated crumpling mode. The compressibility of the system decreases as the aspect ratio of the sheet decreases and the degree of compression increases. The evaluation of stress and curvature distributions of the ribbon further reveals the stress heterogeneity that decreases due to increasing aspect ratio. Our study provides fundamental insights into the size-dependent structural behavior of nanoribbons under crumpling, which is crucial to develop the structure-property relationships towards designing and engineering crumpled matter.

https://symposium.foragerone.com/nd-epscor-2022-state-conference/presentations/37345

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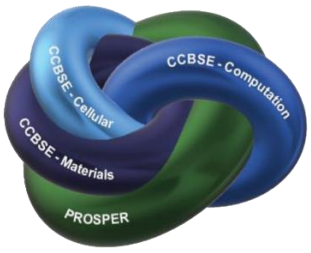
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