



## **2007 WVNano NSF REU Site Multifunctional Nanomaterials Project Descriptions**

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## **Proteomics**

### **Main faculty supervisor and other involved faculty**

Aaron Timperman (Chemistry), Jonathan Cumming (Biology)

### **Goals of the project (for the summer)**

To sequence proteins from sea water.

### **Project description**

Microfluidic and nanofluidic devices are being developed for improved separation and sequencing of proteins to determine their amino acid sequences. These devices will improve our ability to track changes in proteins responsible for the onset of diseases, including cancer, and will be used to find protein biomarkers for disease diagnosis. The REU participant will be involved with the fabrication and use of these devices for protein separation and analysis. The increase in atmospheric carbon dioxide concentrations in the last century is well established. The first step in removal of carbon from the biosphere requires it to be transformed into organic carbon by plants in the oceans. Some of this organic carbon is extraordinarily stable and persists for thousands of years, allowing a large amount of carbon to be stored in dissolved organic carbon. The amount of carbon stored in dissolved organic carbon is significant as it is equal to the total carbon stored in the atmosphere. In spite of its importance, little is known about the chemical structures of dissolved organic carbon in the oceans. In our lab we are characterizing one part of dissolved organic carbon, dissolved proteins, from the oceans and are determining what makes some proteins so stable in the oceans. The REU participant will be involved with the purification, separation, and determination of the amino acid sequence of the proteins using modern mass spectrometry approaches.

### **Experimental/theoretical skills that participant will acquire**

Advanced mass spectrometry, separations, and protein purification

### **Location of the project**

Chemistry Research Labs



## **Electric Fields at a Microfluidic Intersection**

### **Main faculty supervisor and other involved faculty**

Boyd Edwards (Physics), Aaron Timperman (Chemistry)

### **Goals of the project (for the summer)**

To calculate the electric fields at a microfluidic intersection.

### **Project description**

Voltage switching holds promise in lab-on-a-chip devices for analyzing samples of human fluids for disease prevention and cure. Accurate predictions of voltage switching behavior in a microfluidic device requires relies on accurate computations of the electric fields in the microfluidic intersection of the device. Previous predictions rely on simple models of the electric field. The proposed effort will improve the reliability of these predictions.

### **Experimental/theoretical skills that participant will acquire**

Participants will acquire skill using MATLAB and COMSOL Multiphysics software, the leading products for scientific computation and analysis.

### **Location of the project**

Hodges Hall (Department of Physics)



## **Stacking Interactions and Atypical Kinetics of a Cytochrome P450 Protein**

### **Main faculty supervisor and other involved faculty**

**Primary faculty supervisor:** Peter Gannett (Basic Pharmaceutical Sciences)

**Secondary faculty supervisor:** James Lewis (Physics)

### **Goals of the project (for the summer)**

- 1) Quantitate the substrate-effector interactions in the active site of cytochrome P450 2C9 using molecular dynamics trajectories and the Fireball software package.
- 2) Create a predictive model for substrate-effector interactions based on the computational results.

### **Project Description**

Cytochrome P450 2C9 (CYP2C9) is a liver enzyme responsible for the metabolism of 20% of all drugs consumed. Drugs (enzyme substrates) that are metabolized by this enzyme are examined to determine the rate of metabolism. Based on the experimentally determined rate of metabolism, dosages are calculated. However, certain drugs (termed effectors) can accelerate the rate of metabolism of a drug (substrate) and the calculated dose will be too low, with potential negative health effects. Currently, there is no model to predict when a drug will act as an effector and since most people who are taking drugs to treat a disease are taking multiple medications, the potential for substrate-effector interactions is high. Experimentally determining all possible substrate-effector combinations is impractical. Consequently, an computational model is needed. Based on previous molecular dynamics studies, it is likely that a major contributor to substrate-effector interactions is pi-pi stacking. To quantitate these interactions and thus begin to build a predictive model, the computer program Fireball will be used to calculate the interaction energies of the substrate and effector. The results will be correlated with kinetic data with known effectors as well as drugs that have no effect or an inhibitory effect on drug metabolism.

### **Experimental/theoretical skills that participant will acquire**

This project is primarily computational in nature. A participant will become familiar with computational methods used to study chemical and biological systems and the application of these methods to drug design and discovery. In addition, as a model is developed, it may become necessary to experimentally determine the pharmacokinetic parameters of potential effectors derived from the computational model.

### **Location of the project**

Physics (312 Hodges Hall) and Health Sciences Center (HSC, 1128 HSN). (Computer facilities in Physics and HSC and 2033 HSN [wet lab in HSC]).



## Detection of Lactate by a Nanowire-Based Electrochemical Biosensor

### Main faculty supervisor and other involved faculty

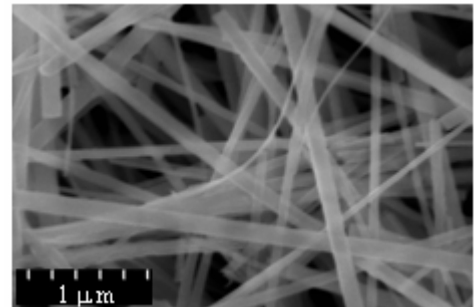
Nick Wu (Mechanical and Aerospace Engineering)

### Goals of the project (for the summer)

Construct a nanowire-based biosensor and test the sensing performance of the sensor.

### Project Description

Enzyme immobilization is critical to the performance of amperometric biosensors, because for the majority of enzymes, their active sites are insulated by the protein matrix of the enzyme, thus blocking the direct electron transfer between the active sites and the electrode. To solve this problem, chemical mediators are usually employed to transduce enzyme activity into an electrical signal. The mediator regenerates the enzyme and itself by exchanging electrons with the enzyme and with the electrode. An alternate strategy for promoting direct electron transfer is to employ nanoparticles that can penetrate the insulating protein matrix, allowing the direct contact between the nanoparticles and the active sites. In the present work, we use titanate nanowires (TNWs) as electron mediators in a lactate biosensor, which transduce enzyme activity via direct electron transfer. TNWs are attractive in immobilization of enzymes in electrochemical biosensors due to their high surface area, chemical inertness, biocompatible, and other excellent properties. Our experiments will provide a base for development of sensitive, rapid and inexpensive lactate biosensors that should find extensive applications in environmental monitoring, food processing, clinical diagnostics, and medical research.



Dispersed titanate nanowires

### Experimental/theoretical skills that participant will acquire

Nanowire fabrication and biomolecular attachment.

### Location of the project

Engineering Sciences Building, Evansdale Campus.



## Large-Area Nano-patterns Fabricated by Nanosphere Lithography

### Main faculty supervisor and other involved faculty

Nick Wu (Mechanical and Aerospace Engineering)

### Goals of the project (for the summer)

To utilize the self-assembly template lithography with electrochemical techniques to fabricate nano-patterns that have potential applications in in photonic devices, optoelectronic device, biosensors, catalysts and high-density magnetic recording devices.

### Project Description

Large-area-ordered two dimensional (2D) nanostructures on the surface have extensive applications in photonic devices, biosensors, catalysts and high-density magnetic recording devices. Future success of 2D nanostructures depends on the availability of facile patterning methods that can scale up at low cost. Commonly used patterning techniques such as photolithography, electron beam lithography, and focused ion beam (FIB) lithography have limitation in fabrication of 2D nanostructures. It is very difficult for the photolithography method to generate features smaller than 100 nm. E-beam and FIB techniques are limited by their low throughput in creating large area nanoscale patterns. Patterning with the self-assembled materials as the templates, such as nanosphere lithography pioneered by Deckman and Van Duyne, is an inexpensive, simple, high-throughput alternative routine for creating periodic nanostructures. In the present work, we will introduce a simple method to overcome the above drawbacks and obtained a large-area ( $\sim\text{cm}^2$ ) well-ordered nanodot array.

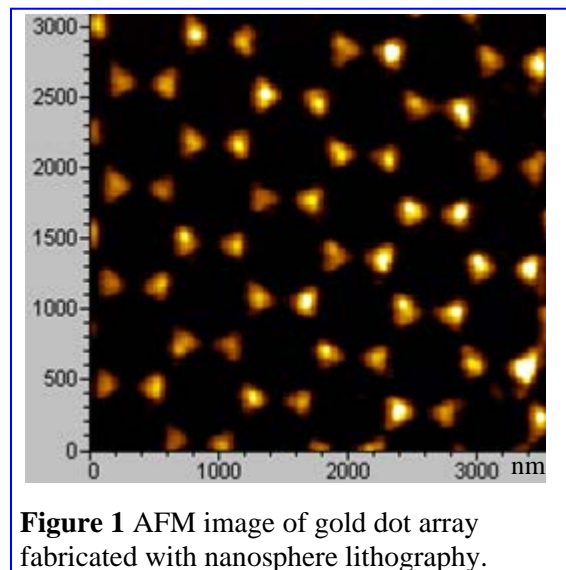


Figure 1 AFM image of gold dot array fabricated with nanosphere lithography.

### Experimental/theoretical skills that participant will acquire

The participant will learn to operate thin film growth equipment used to fabricate the nanostructures, characterize surfaces using atomic force microscopy, and measure the properties of self-assembled nanostructures.

### Location of the project

Engineering Sciences Building, Evansdale Campus.



## **Miniaturized Biotechnology**

### **Main faculty supervisor and other involved faculty**

Lisa Holland (Chemistry), David Lederman (Physics).

### **Goals of the project (for the summer)**

The goal is to introduce the student to a laboratory environment and encourage them to apply biology, chemistry, engineering, and physics coursework to a research project. The student will be encouraged to consider careers in research and will be mentored on the education and training necessary to pursue a career in research.

### **Project Description**

This project involves the implementation of miniaturized flowing stream enzyme cleavage of proteins for analysis by capillary electrophoresis. The REU student will perform protein expression and capillary separations of protein. The student will learn analytical figures of merit, biotechnology, and enzyme kinetics during the summer.

### **Experimental/theoretical skills that participant will acquire**

Record keeping, problem solving, critical thinking, hypothesis testing, gel electrophoresis, protein chemistry, nanotechnology.

### **Location of the project**

Department of Chemistry (351 Chemistry Research Labs).



## **Nanophotonics: Design and Fabrication of Photonic Crystals**

### **Main faculty supervisor and other involved faculty**

Larry Hornak, (Electrical Engineering) (Advisor)

Andrew Cao (Electrical Engineering)

David Lederman (Physics)

### **Goals of the project (for the summer)**

1. Complete the basic design of a 2-D photonic crystal
2. Implement a process for Si PC fabrication
3. E-beam write the PC pattern successfully in PMMA
4. Transfer of the PMMA pattern to silicon
5. Characterize the geometry of the structure

### **Project Description**

Photonic crystals are exciting new structures revolutionizing the way we build devices to control the motion of light. Photonic crystals are designed structures that can control the propagation of light in ways not possible in naturally formed materials. We will use state of the art computer aided design tools to design photonic crystals that will specially designed defects capable of guiding and storing light of specific wavelengths. These structures will be used as building blocks to assemble integrated chip-level systems able to optically detect biological agents that emit at wavelengths matching the photonic crystal's design. We will design and fabricate a photonic crystal (PC) in silicon using electron beam writing with pattern transfer using silicon reactive ion etching.

### **Experimental/theoretical skills that participant will acquire**

- Introduction to optical simulation tools for PC design
- Understanding of integrated fabrication techniques
- Use of electron-beam lithography for PC patterning
- Use of clean room and basic processing for PC fabrication
- Understanding and use of Scanning Electron Microscope (SEM) and Atomic Force Microscope (AFM) for imaging of the PC structure on the micrometer and nanometer scale

### **Location of the project**

Home/office location: Electrical Engineering

Optical design and characterization: Electrical Engineering

E-beam writing: Physics

Imaging: Engineering and Physics



## **Investigation of Aluminum Nitride's Microstructure Effect on the Macroscopic Piezoelectric Properties**

### **Main faculty supervisor and other involved faculty**

Dimitris Korakakis (Electrical Engineering)

David Lederman (Physics)

### **Goals of the project (for the summer)**

The microstructure of AlN thin films will be studied using Atomic Force Microscopy to determine the piezoelectric coefficient with high resolution. The results will be compared to the measurements taken by Doppler Shift Vibrometry.

### **Project Description**

The most common materials used for piezoelectric (PZ) sensors and actuators are Zinc Oxide (ZnO), Lead Zirconate Titanate (PZT) and Aluminum Nitride (AlN). Of these, AlN is the most promising for high temperature applications because of its high thermal stability and no known, to date, transition temperature. However, the PZ coefficient of AlN is about 2 orders of magnitude lower than that of PZT and therefore its applications' potential was seen as limited. AlN films can be grown by Metal Organic Chemical Vapor Deposition (MOCVD), with high crystalline quality, or deposited by reactive sputtering. Both sputtered and MOCVD films exhibit microstructure that has been seen to yield non uniform PZ properties across the film. Recent research has also shown that the apparent PZ coefficient of AlN can be enhanced by designed metal-AlN structures, with a thickness of several nanometers each, which exhibit much higher PZ response when compared to single films. Therefore, to optimize the structure design and improve the quality of the AlN films it is essential that an understanding of the microstructure is developed and correlated to the long range, macroscopic PZ properties of the films.

### **Experimental/theoretical skills that participant will acquire**

The participant will acquire skills in Atomic Force Microscopy and in statistical data analysis of the results. Furthermore, the participants will be able to lay the foundations for developing theoretical models to relate the crystalline or surface structure of the films to the PZ properties.

### **Location of the project**

This project is a joint effort between the Lane Department of Computer Science and Electrical Engineering and the Department of Physics. Most of the experimental work will be carried out in the Department of Physics.



## **Innovative Biomimetic Nanotechnology Coatings for Biomedical Applications**

### **Main faculty supervisor and other involved faculty**

Bingyun Li (Orthopedics, West Virginia University School of Medicine)

### **Goals of the project (for the summer)**

This research project will evaluate *in vitro* the effect of the unique microstructures of polypeptide nanotechnology coatings on cell adhesion, cell proliferation, and cytotoxicity, and their potential applications in rapid fracture healing.

### **Project Description**

The proposed work is *innovative*, because the nanotechnology approach will allow us to modify the current biomedical devices with desired surface properties, which will greatly stimulate osteoblast cell adhesion and therefore to achieve rapid traumatic fracture healing. This project is *important* because trauma is one of the leading causes of loss of life in the U.S.

The student will pursue the following studies:

- Prepare polypeptide biomimetic nanocoatings with unique surface microstructures on stainless steel discs.
- Evaluate *in vitro* cell adhesion and cell proliferation, as well as cytotoxicity of osteoblast cells.

### **Experimental/theoretical skills that participant will acquire**

Cell culture, self-assembly nanotechnology, UV-vis, confocal fluorescent microscopy.

### **Location of the project**

Biomaterials, Bioengineering, and Nanotechnology Laboratory, Department of Orthopedics, WVU Health Sciences Center.



## **Biomimetic Biomineralization of Nanoscale Phosphates**

### **Main faculty supervisor and other involved faculty**

R. Lloyd Carroll (Chemistry)

### **Goals of the project (for the summer)**

- Develop a hydrogel-based diffusion-controlled system for the growth of hydroxyapatite precursors.
- Grow hydroxyapatite precursor minerals and characterize their crystal structure by multiple techniques.
- Grow nanoscale rods of hydroxyapatite precursors and characterize them by XRD and SEM.

### **Project Description**

Living systems have had millennia to optimize the growth processes of biominerals for use as structural components in their systems. Molluscs and other invertebrates use calcium carbonates for protection in their external shells, diatoms and sponges build incredibly complex silica skeletons, and vertebrates have developed the mechanisms to incorporate phosphate-based minerals (such as hydroxyapatite) into bone, providing rigidity and strength. These minerals are produced by the membrane- and protein-controlled reactions of components to form specific crystal forms that are most useful in the biological context. The resulting materials have interesting properties and would be valuable if they can be produced in a carefully controlled manner. We have taken the first steps toward this process with the development of a controlled reaction system for the growth of nanoscale calcite. We would like to extend this work towards other interesting biomineralization products, including hydroxyapatite, and its relatives, octacalcium phosphate and tricalcium phosphate using a hydrogel-based diffusion system, modified with polyelectrolytes to impart selective ion passage to the gel. The polyelectrolyte-modified hydrogel will be used to control the interaction of reactive ions, and force the precipitation reactions to occur at controlled rates on engineered surfaces. The crystals will be characterized by SEM and XRD to identify morphological changes and crystal structure. In addition, we will use polycarbonate track-etched films as nanoscale test-tubes to confine the reaction and template the crystal to a rod shape. These materials may have uses as bone-reconstruction materials, nanoscale mineral sources, or components in nanoscale devices. The techniques that students learn will be applied to other, non-biotic materials, such as semiconductors and metals.

### **Experimental/theoretical skills that participant will acquire**

Students will gain familiarity with wet chemical techniques, electron and optical microscopy techniques, and surface and structural characterization systems.



## **Location of the project**

Experiments will be primarily carried out in Hodges Hall (B-07) and in the Chemistry Research Labs (550/556).

## **Quantum Mechanical Confinement in Ultrathin Magnetic Films**

### **Main faculty supervisor and other involved faculty**

Sergei Urazhdin (Physics), David Lederman (Physics)

### **Goals of the project (for the summer)**

Determine if very thin magnetic films exhibit oscillations of their magnetic/electronic properties due to quantum confinement of the electrons within their thickness.

### **Project Description**

Develop a procedure to deposit ultrathin atomically smooth magnetic (Ni) films by molecular beam epitaxy or sputtering. Determine the surface properties of the films by x-ray scattering and/or RHEED. Determine the dependence of the magnetic properties of the films on their thickness by magnetic and/or magnetoelectronic measurements: SQUID magnetometry and/or anisotropic magnetoresistance. This project explores the idea that the properties of thin films can be tailored by adjusting their thickness when it is comparable to the characteristic wave-vector of the confined electrons.

### **Experimental/theoretical skills that participant will acquire**

Material deposition techniques: sputtering and/or molecular beam epitaxy.  
Analysis techniques: RHEED, SQUID magnetometry and/or magnetoelectronic transport measurements.

### **Location of the project**

Hodges Hall (Department of Physics).



## **Detection of Cancer Marker Proteins Using Microcantilevers**

### **Main faculty supervisor and other involved faculty**

David Lederman (Physics), Lisa Holland (Chemistry), Peter Gannett (Pharmacy), Daniel Flynn (Mary Babb Randolph Cancer Center, West Virginia University School of Medicine)

### **Goals of the project (for the summer)**

Determine if microcantilevers can be used to detect minute amounts of cancer marker proteins.

### **Project Description**

Vascular endothelial growth factor (VEGF) is a protein generated by cancerous tumors that aids them in growing vasculature which in turn enables them to grow. In this project we will develop a VEGF detection device initially based on a piezoelectric driven microcantilever. Selectivity of the system will can be achieved by coating the cantilever with anti-VEGF (VEGF antibody). Exposure of this cantilever system to samples containing VEGF will lead to binding of the VEGF to the anti-VEGF, increase the weight of material on the cantilever and change the resonance frequency. Quantitation will be possible by measuring changes in the resonance frequency (against a calibration curve).

### **Experimental/theoretical skills that participant will acquire**

Atomic force microscopy, chemical functionalization of surfaces.

### **Location of the project**

Hodges Hall (Department of Physics), Chemistry Research Labs.