2013 SURF

summer undergraduate research fellowship

ABSTRACTS

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Table of Contents

Alabama A&M University

Laboratory Instrument Driver for Residential Scale Grid Emulator
Travis Hinton

Smart Grid is a modernized grid that enables bidirectional flows of energy and uses two-way communication and control capabilities that will lead to an array of new functionalities and applications. It is a planned nationwide network that uses information technology to deliver electricity efficiently, reliably, and securely.

NIST requires a Grid Emulator system for testing interoperability of residential scale Smart Grid devices for a wide range of Smart Grid electrical system and network scenarios. The Smart Grid devices include micro grid, Power Conditioning System (PCS), smart meters, and other Smart Grid appliances including thermostats and clothes dryers. This system is to be part of the NIST Smart Grid Interoperability Test Facility and thus requires laboratory instrumentation control of all functions.

The goals of the SURF project are to develop a graphical user interface (GUI) and instrument driver program using the Lab Windows/CVI environment for a programmable AC generator. This programmable AC Generator communicates with the GUI through a general purpose interface bus (GPIB) connection. The program initializes and configures the programmable AC Generator and simulates browning and swelling conditions. The program is also used to produce a grid emulator with controlled waveforms representing specific grid events (e.g., Constant Current, Electromagnetic Interference (EMI) conditions, etc.) that required testing the interoperability of smart grid devices and systems.

Temporal and Spatial Trends of Perfluorinated Compounds in Ringed Seals (Phoca Hispida) from Alaska
Tamika Ragland

Perfluorinated Compounds (PFCs) have been found in at a high level in many marine mammals from the Arctic. Ringed seals (*Phoca hispida*) are a circumpolar marine mammal species that can be found throughout the Arctic Ocean, with the only recognized stock of ringed seals in the United States located in northern Alaska. There are a number of studies examining the accumulation of PFCs in ringed seal samples from Canada and Greenland; however, there are no studies examining the levels of PFCs in tissues collected from the Alaskan Arctic. To better understand the temporal and spatial trends of PFCs in the ringed seal population from Alaska the concentrations of 15 PFCs were measured in 53 ringed seal liver samples banked and collected by the National Institute of Standards and Technology's National Marine Mammal Tissue Bank.

For this project, a previously developed method was used to prepare ringed seal liver samples, calibrants, blanks (water), and Standard Reference Material (SRM) 1947 Lake Michigan Fish Tissue for analysis. The sample preparation included an internal standard addition, a sonication, and a solid phase extraction step. After sample preparation, the ringed seal liver samples, calibrants, blanks, and SRMs were analyzed for PFCs by liquid chromatography-triple quadruple mass spectrometer (LC-MS/MS). After integrating and analyzing the data from the LC-MS/MS, perfluorooctane sulfonate (PFOS) was found to be the major contributor to the total PFCs found in all the ringed seal liver samples. Perfluorononanoic acid (PFNA) and perfluorodecanoic acid (PFDA) were also detected in most of the samples. The ringed seal population examined showed an increase in PFNA ($p<0.05$) over the study period and a relatively constant temporal trend for PFOS. The data mentioned in this talk can help compare and contrast temporal and spatial trends found in ringed seal liver samples from different locations around the world and highlight possible causes for population changes.

<u>Alfred University</u>

All Dressed Up and Somewhere to Go:
A SWCNT-Surfactant MD Study
Daniel Kutzik

Single-walled carbon nanotubes (SWCNTs) are rigid, hollow molecular carbon cylinders noted for their structural properties, as well as their varying electronic and chemical properties that make them appealing for a myriad of advanced technological applications. However, a practical barrier stands between taking full advantage of their varying properties since they are synthesized in large heterogeneous mixtures of abundant lengths and chiralities. Most ongoing research focuses on attacking this barrier by using separation techniques that rely on dispersing aqueous SWCNT species with surfactants to obtain monodisperse tube fractions. Relying on aqueous surfactant-SWCNT solutions, selective SWCNT separation (SSS) may be induced using density gradient ultracentrifugation (DGU) to stratify SWCNT chiralities by density differences or aqueous two-phase extraction (ATPE) to impose a selective aqueous barrier intermediated by dissolved bile salt surfactants and anionic co-surfactants acting on individual SWCNTs.

The dispersion process results in a mixture of colloidal structures in which individual tubes are dispersed and contained in a surfactant shell. Understanding the structure and properties of the SWCNT-surfactant complex at the molecular level, and how this is affected by chirality, is the key to understanding and improving separations processes.

In this project we used molecular dynamics (MD) simulations to study the structure and properties of SWCNT-surfactant colloidal complexes. We tested a number of methods and protocols in order to build an accurate model for simulating SWCNT systems for a variety of bile salt surfactants as well as anionic co-surfactants, components that are widely used and important in experimental separation studies at NIST. In addition, the custom force field parameters developed and used in this work are part of a demonstration project for a Web-hosted smart force-field repository for polymeric and other organic materials called WebFF, which is being developed as a MSED response to the Materials Genome Initiative.

<u>American University</u>

Accelerated Aging of Nuclear Power Plant Cables
Melissa Novy

Cables in nuclear power plants are essential to monitoring the status of the reactor and maintaining safety requirements. Because these cables are subject to a variety of potentially damaging conditions, including temperature, humidity, light, and radiation, it is necessary to monitor their degradation to prevent failures from occurring within the nuclear power plant. Of particular interest are cables that are stored underground, since their location precludes accessibility for maintenance and increases the chance that the cables will come into contact with water. The polymer jackets and insulation of nine different types of cables commonly used in nuclear power plants were characterized by ATR-FTIR spectroscopy, density, and indenter modulus. Then, each of the cables was aged in different environments: 55°C and 75% relative humidity and submerged in water (tap and deionized) at 75°C. The effects of elevated temperature and humidity and exposure to water on the cables' polymer components were monitored on a weekly basis using the above characterization methods. Degraded cables displayed changes in results for each characterization method. These changes depended significantly on the aging conditions and polymeric material used in the cables.

Andrews University

Improved Signal Generation and Acquisition Methods
Thomas Zirkle

NIST calibration services for voltage, power, impedance and phase over the DC to 1 MHz frequency range rely on state of the art signal generation and acquisition techniques. In general, devices with the performance characteristics necessary for these systems are not commercially available. This project involves the design and construction of a single-channel prototype Digital to Analog Converter (DAC) circuit to meet this need.

The primary objectives of this project are the design and implementation of an Infinite Impulse Response (IIR) filter and a Sigma Delta Modulator (SDM) in Field Programmable Gate Array (FPGA) chips. The IIR and SDM will be used in the DAC circuit for interpolation and the actual DAC conversion, respectively. FPGAs were selected for this application due to their low power and high processing rates. Their drawbacks, however, include limited functionality and resources. Therefore, careful consideration must be made as to the design of the logic used to realize the IIR and SDM in order to maximize efficiency with minimal loss in performance. These considerations, as well as the approach to meeting these goals, will be presented in this talk.

Appalachian State University

Development of Calibration Standards for Near Infrared Fluorescence Diagnostic Imaging Systems
Michael Aiken

Several medical imaging technologies developed over the past decade take advantage of the so-called Near-Infrared (NIR) optical tissue window, a region between approximately 700nm and 900nm where optical transmittance within most living tissue is higher. Various emergent technologies operating in the NIR spectral region show great promise as safe, economical in-vivo diagnostic and sensing solutions. Several systems are approaching clinical trial status, in applications such as lymphatic system diagnostic imaging, biomarker enhanced tumor detection, and in-vivo tissue oximetry, to name a few.

Our collaborating group at the University of Texas Health Science Center, led by Dr. Eva Sevick-Muraca, has developed a novel method of non-invasive evaluation of prostatic cancer metastasis, using biomarker-enhanced NIR Fluorescence (NIRF) technology. Currently, lymph nodes are fully removed and dissected in the assessment and prevention process for metastasis, often leading to the painful and unsightly complication of lymphedema. Dr. Sevick-Muraca's method works by using a novel molecule that fluoresces in the NIR only when bound to a specific protein within neoplasms known as an Epithelial Cell Adhesion Molecule (EpCAM). A 785nm laser is used to excite a fluorescent dye present in the biomarker, which is then imaged in real time via a filtered CCD detector. However, in order to quantitatively assess the presence of metastasis, one must be able to evaluate the baseline characteristics of the imaging system in use, and relate these to a known standard in metastatic positive patients. Also, by accurately assessing the sensitivity of the instrumentation used, the minimal amount of NIRF contrast agent can be employed, thereby limiting a patient's exposure to a substance that can be toxic in high doses. This is a crucial factor in allowing clinical trials for this promising new technology to proceed.

Presently, no standardized phantoms or reference instruments exist to evaluate the optical performance of NIRF imaging systems, or to quantify fluorescent intensity measurements for clinical purposes.

U. Texas has developed a candidate phantom using fluorescent nanoparticles known as quantum dots (Qdots), dispersed within a mixture of titanium dioxide pigment and epoxy. Its design attempts to accurately mimic the optical scattering that occurs deep within living tissue across the NIR spectral range.

Our research at NIST aims to provide a repeatable methodology for calibrating field instrumentation such as clinical imagers and to provide a path for future SI traceable optical clinical measurements.

We are concurrently evaluating a suite of candidate phantoms provided to us by U. Texas for suitability as a materials-based calibration standard using a laboratory grade spectroradiometer, and a separately configured filtered radiometer that can be set up to mimic a clinical measurement configuration.

Measuring Absorbed Radiation Dose in Water Using Optical Interferometry

Nikolai Hesterberg

Accurate calibration of cancer-treatment radiation devices is essential for quality assurance in hospitals and cancer treatment clinics. In order to accomplish this calibration, the dose being delivered to the human body must be measured. Currently, there is no suitable approach to base calibration standards on DNA damage of tissue. Instead, calibration standards are based on energy deposition in a simpler tissue-analogue material, water. Water absorbs radiation at a similar rate as human flesh, and the dose can be measured as a temperature increase in the water. This brings up many challenges because the temperature changes associated with therapy level doses are on the scale of a few milliKelvin (mK), and any probe or vessel within the water will change the rate of absorption. My research evaluated a new method of measuring such small temperature changes using optical interferometry. The method used a Michelson interferometer with a HeNe laser and one arm going through air with a fixed optical path length and the other passing through the container of water. As the water is irradiated, the water temperature increases and the index of refraction changes. The change in the index of refraction causes a difference in the speed at which the photons pass through the water, causing the optical path length to change. This causes the projected interference pattern of the interferometer to change, and this rate of change is directly related to the temperature change of the water. By projecting the interference pattern onto a photo detector, it is possible to get an electronic signal showing changes in the interference pattern. The detector signal can then be used to calculate how much the temperature has changed. In my research on the technique, we were able to measure temperature changes down to a few mK, and identified many sources of instability in the measurements. In theory, this interferometry should allow measurement of temperature changes down to sub mK levels, which is essential considering that a typical radiation source depositing 1 gray per minute is only increasing the temperature of the water by .25 mK per minute.

Stellar Photometry: Calibration of Stars
Zachary Pruett

For eleven nights from June 17-28, 2013 at the Fredrick Lawrence Whipple Observatory on Mount Hopkins, Tucson, Arizona, four standard stars and a manmade calibration "star," were observed both photometrically and spectroscopically. The goal was to make an SI-traceable measurement of the light from each star at the top of the Earth's atmosphere. Stars observed include: HIP64238, HIP77622, HIP97980, and Vega. Photometric observations were taken using filters with center wavelengths at 410nm, 488nm, 500nm, 530nm, 615nm, 585nm, 860nm, 780nm, and 380nm, 410nm, 460nm, 540nm, 630nm, 760nm, 860nm, and 935nm on two different telescope setups. Spectroscopy was performed with a third telescope. A 2-inch integrating sphere illuminated by a 10W quartz tungsten halogen lamp served as the manmade "star" and was placed on the summit, approximately 800 meters from the observing site at the ridge of the mountain. The output of the artificial star was measured at close range on the summit with a calibrated spectrometer. A separate apparatus measured the light lost between the summit and the ridge.

We were able to determine the relative apparent brightness of the stars at zero air masses by fitting a curve to the relative apparent brightness of the stars as they change due to absorption and scattering in the atmosphere throughout the course of the night and then extrapolating to zero air masses. (In other words, a curve in relative irradiance versus optical depth in air masses was generated and used to calculate the irradiance at zero air masses.) We were then able to put a calibration in absolute units on the irradiance of each star by measuring the artificial "star" of known output to scale the results of the measured stars.

Arizona State University

Characterization of High Density Plasma Chemical Vapor Deposition Process
Osama Khalil

The Center for Nanoscale Science and Technology's nanofabrication facility at NIST replaced the plasma enhanced chemical vapor deposition system (PECVD) with a new high density plasma chemical vapor deposition tool (HDPCVD) in May 2013. The PECVD experiences high traffic from NanoFab users, because of its convenience in depositing a variety of thin dielectric layers on substrates in a matter of a few minutes. The PlasmaTherm HDPCVD is expected to deposit silicon oxide and silicon nitride on silicon at temperatures 200°C lower and deposition rates one order of magnitude greater than the PECVD tool it replaced in the NanoFab. The manufacturer of the tool has provided baseline recipes that I used as a starting point in optimizing the chemical process design. My work is meant to provide NanoFab users with response surfaces and regression models that can be used to alter baseline recipes on the HDPCVD system to tune deposition rate, film stress, index of refraction, thickness non-uniformity, and buffered oxide etch rate as desired.

Six recipe factors were manipulated in two half-factorial central composite response surface experimental design (one for oxides and one for nitrides), including silane volumetric flow rate, the ratio between silane and oxygen flow rates, argon flow rate, processing chamber pressure, biasing power, and inductively coupled plasma power (ICP).

In addition to characterizing the process, I have contributed to the general user's manual, created a compact user's guide to help familiarize new users to the tool, and modeled the chemical reaction kinetics of the deposition process.

A Really Hot Way to Measure Airflow
Jenna Lynch

Heat pumps and air conditioners are tested at standard indoor and outdoor temperature conditions to determine their published rated cooling capacity and efficiency. To do these standard tests, the indoor unit that circulates the air within a home must be connected to an airflow measurement device. This device normally consists of large nozzles through which the air flows and experiences a rapid acceleration and pressure drop. By measuring this pressure drop the airflow rate in cubic feet per minute (or meters cubed per minute) may be calculated. These nozzle chambers are very good for measuring airflow, but like any other measurement that is important, a secondary way to verify the measurement is always desirable. To verify the nozzle chambers measured airflow, a secondary energy balance method may be used to determine airflow. This method involves connecting the nozzle chamber in series with an electrically heated duct section so that the same air flows through both devices. The air flowing through the heated duct section experiences a temperature rise; measuring the temperature rise, air temperature, air humidity, and power input to the heater allows calculation of the airflow rate based upon an energy balance. The two devices connected in series should ideally produce airflow rate measurement results that are within plus or minus 2%. This talk discusses the construction of this heated duct secondary airflow measurement device, the uncertainty of the heated duct airflow measurement, and the results produced when connected and compared to a nozzle chamber airflow measurement.

Correlations Between Fullerene Miscibiity and Organic Photovoltaic Device Performance
Stuart Ness

Significant interest has been developed in the production of organic (plastic) solar cells that can be fabricated by low cost, roll-to-roll technologies. Device performance is critically dependent on the development of structures that support optimal charge separation (short circuit current Jsc) and device voltage (Voc). Predictive guidelines for Voc exist, based on the electron affinity and ionization potential of the polymer donor and fullerene acceptor. However, fullerene acceptors designed for high Voc often result in devices with unacceptably poor Jsc. A predictive model for the poor performance of some polymer/fullerene pairs is not available. It has been hypothesized that in some cases, poor performance can be related to the miscibility of the fullerene in the polymer matrix.

We created devices utilizing a newly introduced photovoltaic polymer, PCDTBT, which the literature has shown to make high-performance devices when paired with the fullerene PCBM-71. NIST has recently acquired miscibility data for PCDTBT with four fullerenes: PCBM–71, PCBM-61, bis–PCBM, and ICBA, all of which have formed good devices with the early generation polymer P3HT. This summer, we measured performance of PCDTBT devices made with all four fullerenes. Device performance is critically dependant on the mole ratio of polymer to fullerene and the film thickness. Based on early tests of PCBM-71, we standardized our films to ~80nm. For each fullerene, three loadings were explored. The devices where made in the conventional geometry: ITO anode, PEDOT hole injection layer, polymer/fullerene active layer, Ca electron injection layer, and finally the Al cathode. To create our thin film photocells, the bulk heterojunction was via blade coating, a method that much more closely resembles industrial flow coating processes than traditional spin coating.

The four fullerenes differ in miscibility by about a factor of three, with PCBM-61 and bis-PCBM being much more miscible than ICBA and PCBM-71. The efficiency data we have acquired will allow the role of miscibility in determining device morphology performance to be rigorously tested.

Atomic Spectra of Iron Group Elements: Looking at the Universe Through Atoms

Jacob Ward

Many astronomical observations have utilized atomic spectrometers for precise data collection and interpretation. Instruments placed within satellites, such as the Hubble Space Telescope, allow astrophysicists to determine multiple characteristics of astronomical bodies such as composition and velocity by creating wavelength and line strength lists for each line in the element's spectra. Among the most prevalent groups of elements found in astronomy research, especially in solar objects, is that of the iron group. Recent publications by Craig Sansonetti and Gillian Nave have produced numerous and accurate standards for the spectra of singly ionized iron and chromium. Other portions of the element group, however, contain line list standards that have been neglected since the 1950's. In particular, singly-ionized manganese wavelengths contain uncertainties that are incapable of providing the accuracy needed to interpret modern astrophysical observations in stellar evolution and supernovae.

Using the NIST 10.7 meter normal incidence spectrometer, this project analyzes the spectra of singly ionized manganese in the vacuum ultra violet wavelength region (500 – 2400 Å). In combination with the normal incidence spectrometer, a hollow cathode light source was used to excite a manganese cathode with stable high voltages of 700-750 V and average currents of 1.5 amps.

The spectra were collected in three manners. A combination of two types of photographic plates and one type of phosphor image plate was used to collect the resulting spectra from the spectrometer. The available photographic plates, Kodak SWR plates and Ilford Q plates, date to the early two thousands and thus, have degraded in sensitivity and are no longer commercially available. The need for large area collection sources, not available with the small CCD sources, has warranted the continued use of photographic plates and, although phosphor image plates have been proven valuable, the photographic plates have significantly higher resolution. Consequently, experiments were conducted to determine if development techniques were capable of partially restoring the plates to their previous quality. Through these tests, promising developing techniques have been identified that have restored the plates to usable conditions. In addition, wavelength regions have been identified for each type of plate in which the sensitivity and quality of the plate is at its peak.

Augsburg College

Benchmarking the Detection Threshold, Saturation Limit, Linear Dynamic Range, and the Intensity Calibration for a Widefield Fluorescence Microscope using Fluorescent Glass Reference Materials

Standard benchmarking methods are needed to assure fluorescence microscope performance and to calibrate data between different imaging systems. We have developed a simple strategy using fluorescent glass to measure the analytical detection performance of a fluorescent microscope. Photostable and uniform fluorescent glass is used as a reference material for benchmarking the performance metrics, which allows for control charting of the instrument performance over time. In this study we evaluated uranyl oxide glass and commercially available Schott 475GG glass as candidate glass reference materials. The procedure for benchmarking the analytical performance normalizes for differences in magnification, physical pixel sizes of the detectors, and bit depths of the image data which allows the analytical metrics to be compared over a wide range of instruments. Using Micro-Manager, open-source microscopy software, a computer program has been developed which automates the procedure and returns four different benchmarking parameters – detection threshold, saturation, linear dynamic range, and intensity calibration. We have tested the program by measuring and verifying the effects systematic changes to a microscope have on the benchmarking parameters. The goal of this work is to provide the fluorescence microscope with reference materials and protocols for evaluation and validation of fluorescent microscope performance.

Bates College

Zeta Potential and Particle size Analysis of Hydrating Cement Solutions

Joanna Moody

It is now well understood that cement reacts when mixed with water, binding together concrete mixtures. It is important, that these cement particles remain dispersed throughout the concrete mixture in order to bind and hydrate evenly. This study follows the electroacoustic behavior of the early hydration reaction in cement and water solutions to better understand how this reaction changes the physical and electrical properties of the cement particles. The cement particle size and zeta potential are recorded over time as hydrates form on the surface of the particles in solution. The zeta potential is an index of the magnitude of the interaction between two colloidal particles and its value can be used to characterize the stability of the particle dispersion in solution. In addition, the cement and water reactions are studied under various treatments of commonly manufactured dispersing agents, called either superplasticizers or high-range water reducing admixture (HRWRA). These chemical additives further stabilize the hydration reaction by creating a combination of steric barriers (more pronounced for polycarboxylate types) and electrostatic barriers (more pronounced for sulfonate types). Increased barrier between cement particles in water is important as it reduces the chance that these particles will flocculate or sediment out of solution. For concrete, this reduced flocculation, or in other words more stable dispersion of cement particles, means a more even binding and hydration that results in greater strength, increased workability and reduced risk of cracking.

Boise State University

EBSD Strain Measurements of $Si_{1-x}Ge_x$ Thin Films on SI Chips for Reference Material Development

Koyuki Fritchman

High resolution electron back-scatter diffraction (HR-EBSD) is an evolving technique for measuring lattice strains and rotations in crystalline materials. Currently, there is no standard or reference material that can be used to verify the accuracy of a particular experimental setup and analysis method. Thus, a NIST reference material (RM) that has a known strain level is being developed as a standard for EBSD equipment, with particular applications in the microelectronics industry.

SiGe and Si are common semiconducting materials which are being investigated for reference material development. In this study, two different compositions of SiGe thin film were deposited perfectly epitaxially onto Si wafers and then analyzed. The various SiGe thin film compositions were deposited onto the Si wafer by industrial collaborators, and scientists at NIST designed and mapped the pattern that was fabricated in the nanofabrication laboratory. A parametric study of strain measurements using the EBSD technique on the Scanning Electron Microscope (SEM) was utilized for evaluation of strain measurements on different SiGe patterns. Both Si and SiGe have diamond cubic crystal structures; however, when SiGe is deposited epitaxially onto the Si substrate, it is compressed to maintain perfect coherency at the Si-SiGe interface resulting in a tetragonal lattice distortion. This lattice distortion exerts a strain which is measured using the shifts of the EBSD patterns. The accelerating voltage was the only SEM parameter modified, while in the data analysis software the reference pattern, regions of interest (ROI), and high frequency filter settings were manipulated to analyze the effect of these parameters on strain measurements. Cross Court 3 strain measurement software was used to cross-correlate Si and SiGe EBSD patterns collected using the EBSD detector on the SEM. Through extensive analysis, it has been found that the accelerating voltage has a large effect on strain measurement between 10 and 20 kV due to sharpness of patterns collected and electron penetration through the thin film; much smaller strain differences were found between 20 kV and 30 kV data collection. As a result of the study, it is recommended that data be collected at a minimum of 20 kV. In addition, high frequency filter settings have a 0.03% to 2.68% relative effect on the EBSD strain measurement, the ROI sizes have up to an 8.44% relative variation when measuring tetragonal strain in SiGe, and the reference pattern selected only has noticeable effects on multi-line scans and not on single line scans. The recommended high frequency cut-off filter setting is between 20 and 30, which is in agreement with the lowest high frequency filter setting variation of 0.03%. The parametric study will be used as a reference for industry to select the proper parameters to calibrate EBSD and XRD equipment using this NIST RM. Time permitting, data may also be presented on the partially epitaxial SiGe films.

Captivating Science: Computational Studies of the Carbon Capture Material HKUST-1

Eric B. Nelson

The rising level of atmospheric carbon dioxide is one of the largest concerns in our society today, for reasons both economic and health-centered. These emissions are produced predominately from the combustion of coal, oil and natural gases (ca. 80% of CO_2 emissions worldwide), which are projected to rapidly increase due to global economic development. [S. Energy Policy 2007, 35, 5938] In June 2009, the U.S. House of Representatives passed the American Clean Energy and Security Act, which proposes economy-wide CO_2 reduction goals by 2050 of 83% below 2005's production levels. Metal-organic framework (MOF) materials are a likely candidate for capturing CO_2 more efficiently than current technologies. Computational work that can accurately predict structure-property relationships in MOF materials would substantially reduce the development time for materials with desired properties. The focus of this study is to refine previous studies on HKUST-1 (CuBTC), a nanoporous material with exposed Cu sites that has a high CO_2 adsorption capacity. HKUST-1 is one of the most studied MOFs for adsorption and desorption properties; however, less is known about its interactions with sorbate molecules. Previous work has shown that it is very difficult to calculate the sorption geometry and energetics for water sorption on HKUST-1. The study uses density functional theory (DFT) calculations at various levels of approximation to study HKUST-1. The experimental structure and bandgap of the related material malachite ($Cu_2(CO_3)(OH)$) were used as a test bed for optimizing DFT parameters and then applied to HKUST-1. Preliminary results are encouraging, and suggest that the so-called "Hybrid" density functional theory approach is required for these Cu-containing systems. Final results from these findings are to be compared with experimental values and used as a benchmark for further theoretical studies.

Crystal Chemistry and Crystallography of Potential Thermoelectric Perovskites
Kevin R. Talley

High energy cost and greenhouse gas emissions are of growing concern to our society. These concerns have driven the research and development of waste energy recovery systems. Thermoelectric materials are useful in energy conversion applications due to their ability to produce an electric potential when exposed to a temperature gradient. The Seebeck coefficient, S, is defined as the voltage generated per degree of temperature difference and has a great influence in determining the conversion efficiency of a material. Therefore, the thermoelectric potential of a material can be determined by screening the Seebeck coefficient. As perovskite ceramics are potential thermoelectric materials, an investigation into the structure property relationships of these systems will aid in the engineering of new thermoelectric materials.

In this study, six thermoelectric oxide perovskites in the series $R(Co_{.75}M_{.25})O_3$, where R=La, Pr, Nd, and M=Fe, Ni, were synthesized by means of high temperature solid state reactions. Phase purity was verified by X-ray powder diffraction. The crystal chemistry and crystallography of each compound was investigated using powder neutron diffraction and the Rietveld refinement technique. Neutron diffraction showed the existence of two different crystal systems, namely, rhombohedral ($R\overline{3}c$) for R=La and orthorhombic (*Pnma*) for R=Pr, Nd. A possible monoclinic structure for R=La (according to the recent literature data for $LaCoO_3$) was ruled out through low temperature powder neutron diffraction studies. Electron diffraction was used to examine the possible existence of a superlattice. To study strain and structural distortions in these two series of compounds, the bond valence sum of the lanthanide and transition metal (Co, M) sites, and the tilting of the $(Co,M)O_6$ octahedra were examined. The degree of octahedral distortion in these compounds was found to be correlated with the lanthanide ionic size, $r(R^{3+})$; the smaller the $r(R^{3+})$ value, the greater the distortion. The Seebeck coefficients (screened using a custom NIST Seebeck coefficient screening apparatus) and structural distortions of these compounds were compared to those of the undoped $RCoO_3$ analogs.

<u>Brown University</u>

A Novel Memory-Efficient Method for Visualizing Large Stitched Images
Anson Rosenthal

To visualize the large stitched images that arise in optical microscopy, previous approaches leveraging technologies such as Microsoft Deep Zoom have required that the image of the entire plate be reconstructed at full resolution as preprocessing for the visualization application. These methods do not scale well with the current advances in acquisition methodology - the memory footprint of such a large, high-resolution image in RAM is significant for many standard workstations in the typical case (~6GB), and exceeds that of even specialized machines in the case of cutting-edge research (~196GB).

Reasoning that such large acquisitions are 1) often impossible to display at full detail, 2) impossible to interpret in their entirety at full resolution, and 3) sparse in terms of interesting data, we have developed an abstraction that provides the user and other programs with access to the full reconstructed image without incurring the memory cost of actually constructing it. The crux of this abstraction is deferring the composing and blending of image tiles to runtime instead of the preprocessing stage, similar in spirit to how, at runtime, our method and current approaches defer the loading of image tiles into memory until they are requested to display the user's current viewport.

We have implemented this design in Java and developed a convenient user interface for viewing both stitched images and stitched image "movies" along with tools for exporting ROIs for further processing. We have also integrated it with the ITL's Image Stitching Plugin to be distributed for use with the ImageJ/Fiji image processing library.

Carnegie Mellon University

Creating a Test Infrastructure for Atomistic Simulations of Materials
Robert Buarque de Macedo

Development of new materials is essential to increasing the prosperity of our nation and the world. However, the development of these materials is traditionally expensive and time-consuming. One way to reduce costs is to create computational models of these materials, and to test these digital models rather than experimenting on the physical substance. Molecular dynamics is a type of atomistic simulation that has growing usage in materials development. However, all molecular dynamics simulations are based on a mathematical relationship that approximates the forces on atoms. This mathematical formula is named the interatomic potential, or force field. Multiple different potentials have been developed for elements and alloys, and it can be difficult for engineers to know which potential will be appropriate for their simulation. We will discuss the creation of an infrastructure for rapid and reproducible potentials testing that is intended to help engineers decide which potential to use. This infrastructure is part of the NIST interatomic potentials repository project. For this project, we created automated programs in iPython notebooks which would run multiple parallel molecular dynamics simulations, store the data in HDF5 files, and present the results on a web page. Our efforts will help scientists and engineers more easily use molecular dynamics simulations.

A Bayesian Approach to Crystal Structure Refinement
Dylan Quintana

Neutron diffraction is a useful technique for uncovering the structure of materials, especially those exhibiting magnetic properties or containing lighter elements. Modern-day diffraction experiments involve the measurement of a diffraction pattern with a neutron scattering instrument followed by computer refinement of a postulated crystal structure. The refinement process aims to minimize the difference between the experimental diffraction pattern and a pattern generated from predicted atomic positions by altering the structural model until it is consistent with the collected data. However, refinement is a delicate task: there may be dozens of independent parameters necessary to model even slightly complex structures, and the process is at risk of yielding a structure corresponding to a local minimum in the difference rather than the best overall fit.

To overcome these deficiencies of traditional refinement, global optimization procedures were applied to neutron diffraction data. This should decrease the chances of getting stuck on a suboptimal structure. The goal of global fitting was realized by combining the diffraction computations of the Crystallographic Fortran Modules Library (CrysFML) with the fitting routines provided by the Bayesian Uncertainty Modeling of Parametric Systems (Bumps) program. Developing an interface between the two required calling CrysFML functions (written in Fortran 90) from within a Python script. The resulting program is capable of generating neutron diffraction patterns for both magnetic and non-magnetic structures, and uses these patterns to refine the crystal structures of materials in neutron diffraction experiments. After rigorous testing against materials with known structures and diffraction patterns, the program was used to determine the magnetic structure of a new multiferroic material, lutetium ferrite, $LuFeO_3$.

Fabrication of Nanoporous Aluminum Oxide Films
Graham Spicer

The study of protein structure remains one of the largest challenges in biology today. Many proteins cannot be crystallized, so a traditional method of x-ray diffraction cannot be used to determine structure. However, small-angle neutron scattering can be used to provide important structural information of proteins and other large molecules, provided they be similarly oriented. We experimented with the fabrication of self-ordered nanoporous anodic alumina films that can be tailored to constrain different molecules with proper orientation. Procedures were developed to create through-hole porous films having self-ordered pores of diameter 30-70 nm. Films were imaged in an environmental scanning electron microscope, and results will be discussed.

Central Washington University

Co-W-Al Isothermal Analysis
Richard Grist

The discovery of the gamma-gamma' two-phase region in the Co-W-Al ternary alloy system has developed much interest due to its comparable structure in current Ni-based superalloys. This two-phase microstructure is what gives Ni-based superalloys high temperature strength and creep resistance. Due to their higher melting temperatures and comparable high temperature mechanical properties, alloys based on the Co-W-Al system show potential as a replacement for current Ni-based superalloys used in high temperature turbine applications such as engines and power generators. If implemented, a Co-based superalloy could potentially allow a turbine to operate at higher temperatures and achieve greater efficiency thus lowering operating costs and increasing performance. For eventual production and alloying, there must be a greater understanding of the thermodynamics and phase equilibria of the Co-W-Al ternary; with most experimental work having been performed at 1173K there has been very limited examination of other temperatures.

This work is focused on determining the microstructure present in Co-W-Al melt spun ribbons of varying compositions to determine the phase equilibria for annealing at 1273K. These samples were analyzed by using x-ray diffraction, field-emission scanning electron microscopy and electron dispersive x-ray spectroscopy to determine which phases are present, the composition of each phase, and overall composition of each ribbon. At this temperature the findings show the L12 gamma' phase is not stable as is expected; but a new Laves phase is observed that has not yet been reported anywhere in literature for this system. This information combined with the previously known phases of gamma, B2, DO19, and mu allows us to begin developing an isothermal section at 1273K in the Co-rich corner of Co-W-Al ternary systems.

City College of New York

Evaluating Smoldering Ignition Performance of Barrier Fabrics (BF)
Zineb Bouizy

This work is a part of large project that aims to reduce residential fires by reducing flammability of soft furnishing products. One of the objectives of this project was to evaluate smoldering ignition performance of Barrier Fabrics (BF). Barrier fabrics are textile materials used in the soft furnishing products to prevent or delay direct flame impingement and heat transfer from burning cover fabric to core cushioning components. Twenty Barrier fabrics were tested in the mock up configuration. The mock up assembly consists of a wooden frame, standard polyurethane foam (SPUF) substrate, barrier fabric and cover fabric (CF). A lighted, smoldering cigarette is used as an ignition source. Commercially available barrier fabrics were tested. Variety of textile structures including highloft, nonwoven battings, knitted, and woven structures used in a variety of soft furnishings were tested in triplicates and analyzed for their smoldering ignitability in terms of char length and mass loss. Physical properties of BFs including area density, bulk density, and air permeability were also studied. BFs were testes with and without the cover fabric. The cover fabric chosen for testing smoldering ignitability of BF was a smolder prone fabric.

Most BFs tested with CF show significant mass loss and were critical in term of the char length of both, the BFs and the Foam. The weight loss range from was 0-30.73% and the char lengths on BFs varied from 63-200 mm. It was observed that air permeability of the BF has significant impact on smoldering ignitability of the mock-up assembly.

The BFs tested without CF have negligible mass loss and the char length of the BFs was about the size of the cigarette. In most cases, the tests were stopped before finishing the duration of the test (45 min), as a result of the cigarette being burned completely and extinguished, and no more smoke. This study suggests that the BFs with high area density and air permeability fail to prevent heat transfer from smoldering CF to the foam.

Polyester battings were placed between BF and CF since large amount of heat from smoldering ignition source is consumed in melting polyester fibers. This essentially prevents heat transfer to BF and limits smolder propagation.

Hole and Electron Internal Photoemission of MOS Devices
Jing Chen

Internal Photoemission (IPE) Spectroscopy and Spectroscopic Ellipsometry (SE) are the important metrology tools for characterizing the electric band structure of metal-insulator-semiconductor (MIS) devices. It is necessary to investigate the band alignment of MIS in order to avoid the unnecessary leakage current in MOSFET devices and control TFET performances.

IPE spectroscopy is a robust measurement technique to determine the electron and hole barrier heights at metal-insulator and semiconductor-insulator interfaces. By shining a monochromatic light on MIS device, electrons can be excited from the valence band of the semiconductor or from the metal Fermi level to the conduction band of the insulator over the barrier height at the interface. The photon energy giving rise to the transition threshold determines the barrier height. The same process can occur for hole injection from conduction band of the semiconductor or the Fermi level to the valence band of the insulator. However, the latter process has been shown to be difficult to observe due to the overwhelming electron ejection. In other words, what makes it difficult of measuring the hole's barrier height at both interfaces is that the electron density in metal and semiconductor is much higher than hole density such that the hole photocurrent becomes negligible and harder to determine. As a solution to that, graphene, the monolayer material is used to replace metal in order to determine the hole injection. Since there will be tiny amount of electrons emitting from graphene, it is easier to investigate the hole injection at the insulator/semiconductor interface. As a complementary technique, SE is a powerful technique to measure the thickness, band-gap, and optical properties of the involved insulator and semiconductor layers. By combining the barrier heights and band gaps determined by IPE and SE respectively, one can arrive at a complete band alignment of MOS devices.

The goal for my SURF internship is to fabricate MOS structures including metal/SiO2/Si and graphene/Al2O3/high mobility channel substrate (GaAs and InP) and to perform IPE and SE on theses structures to determine their interface band offsets. The research will focus on the hole injections in group III-V high mobility substrate. It is expected at the end of the internship, I will be able to derive a completed band alignment of these structures and demonstrate that IPE with graphene as a semitransparent electrode will enable a complete band alignment measurement and thus can be extended to apply to other technologically important materials and structures.

Electrical Transport Measurements of Molecular Layers Using Eutectic Gallium Indium

Marilyn Gauthier

Due to the miniaturization of technology, Aviram and Ratner introduced molecular electronics where they envisioned that molecules would replace macroscopic circuit elements. Other than the molecules being small, molecules are appealing because they can have many different compositions. However, there are some challenges in forming electrical contact to a molecular layer without destroying them or forming electrical filaments through pinholes. Some techniques of forming contacts to the molecular layer include: thermal evaporation, application of a conducting polymer on top of the molecular layer, and use of a liquid metal. Thermal evaporation onto a molecular layer ensures contact but can damage the molecules. The use of a conductive polymer prevents metal filaments from forming, but is unstable. Mercury has been widely used as liquid metal contact for molecular layers, but it is toxic. Eutectic Gallium Indium (E-GaIn) is a liquid metal and is non-toxic. E-GaIn makes non-damaging contacts; it can be molded to conical shapes. It is commercially available and can be used with a syringe. Therefore, we pursued E-GaIn in these experiments to study the electron transport through molecular layers.

The goal of the research is to measure how different molecules affect electron transport. The project that I'm a part of is aiding the development of E-GaIn-based electrical measurement metrology. I investigated the electron transport through a molecular layer – measuring the current from the E-GaIn, through different aliphatic thiol molecules of varying lengths, to the substrate (silicon, gold, and patterned gold wells). Some of the challenges in our setup include determining the contact area for the current density, abrupt changes to the E-GaIn tip during the measurements can alter the data easily. Sample aging between octadecanethiol and hexadecanethiol differs drastically between the two despite having similar lengths. These measurements would help compare electron transport measurements derived from other fabrication methods.

College of the Holy Cross

Analysis of Biodiesel Using Comprehensive Two-Dimensional Gas Chromatography (GCxGC)

Julian Goding

In the search for alternative fuels, biodiesel fuels are being blended with conventional petro-diesel fuels. The main components in biodiesels, fatty acid methyl esters (FAMEs), vary from feedstock to feedstock. These feedstocks differ in FAME concentrations and which FAMEs they contain. These complex blends can be analyzed using comprehensive two-dimensional gas chromatography with time-of-flight mass spectrometry (GCxGC TOF-MS). For this project, various diesel and biodiesel samples were blended and analyzed. The fatty acid methyl esters (FAMES) present in biodiesels were separated and identified from the petro-diesel components. Principal Component Analysis was used during this study and results clearly indicate grouping of blends depending on the biodiesel feedstock. Unknown blends were also analyzed to determine if the biodiesel feedstock can be determined.

Colorado School of Mines

Modeling Dynamic Elasticity in Dynamic Force Calibration

Aaron Glick

Mechanical forces are experimentally measured with force transducers, which output voltage signals proportional to the applied forces. For static force transducers, calibration methods have been established that calibrate devices to uncertainties on the order of $5 \cdot 10^{-6}$. Currently, dynamic force transducers, which measure forces that vary with time, use the same static methods of calibration; although, due to the dynamic nature of the system, these static calibrations cannot achieve the same accuracies. It is our objective to establish a dynamic calibration method used to calibrate dynamic force transducers more effectively, by designing and simulating a mass oscillating with a prescribed sinusoidal force.

Essentially, the method boils down to Newton's Second Law: for a known calibration mass, accelerations are collected using interferometry to calculate the experimental force applied. However, in order to use this method, it is necessary to determine the variation of experimental force measured (from a point on the surface of the mass) compared to the total integrated force (over the entire volume) to minimize calibration uncertainty. As with static force transducers, contributions from factors such as air pressure and surface drag must be considered to obtain small uncertainties. Additionally, wave propagation, interference of displacement waves, and non-uniform body accelerations among other factors complicate the modeling of the dynamic case.

Largely due to the fact that Navier's Equation (which describes the displacement of the mass) does not have a 3D analytic solution, theoretical solutions must be determined numerically. Through finite element analysis, we have created a model that describes the theoretical motion of the mass during the calibration process, to be used as a basis for comparison to experimental data. Together, the calibration device built and the model solutions derived serve as the foundation of a proposed standard for dynamic force calibration.

In this talk I will discuss the simulation parameters which have been determined to produce correct theoretical results, analyze the limitations of this model, and subsequently describe the calibration device built to calibrate dynamic force transducers.

Development of a Deep-Level Transient Spectroscopy Data Acquisition Method for Characterization of Photovoltaics

Timothy Straley

The development of thin film solar cells has been an important contribution to the field of renewable energy and will likely play an increasingly significant role in the future as we face larger energy demands. However, further improvement of efficiency and performance of photovoltaic devices can benefit greatly from our ability to characterize these solar cells on length scales closer to the grain sizes of the materials. Deep-level transient spectroscopy (DLTS) is a powerful method used to study charge carrier traps in semi-conductors on a macro-scale. This technique works by disturbing the depletion region of a solar cell using a voltage pulse, and then measuring the capacitance change that results from charge carriers returning to the steady state after thermal emission from the traps. This project was developed in order to explore the extension of the conventional DLTS to smaller length scales, and to potentially derive techniques that can be used on a single grain in order to gain a better understanding of how grain sizes and grain boundaries influence the productivity of solar cells.

The first stage in accomplishing this task was to create a custom circuit bridge to balance stray signals and currents associated with other circuit elements and not with the transient capacitance that is typically measured in DLTS. A set of programs developed with LabView and custom instrument drivers have been designed to work together to perform this task. Second, we explored the limits of DLTS scaling to small sample volumes. Typically, DLTS has only been used to study macro-scale devices, and not micro-scale components of these devices. Finally, we study the current transients at different temperatures comparing these with the DLTS signals. The goal is to identify the conditions where current dynamics carry the information on the local trap filling. While measuring the capacitance of nanoscale devices is challenging, current-voltage measurements are much more easily performed. After confirming that the current measurements on smaller length scales result in effective characterization of deep traps, the technique will be used to characterize various thin film solar cells and their grains. Such data can help to identify the microscopic origin of the deficiencies of the current technologies as well as assist in developing new thin-film materials for PV applications.

Cornell University

Design and Fabrication of a Nano-Scale Cantilever for the Atomic Force Microscope

Noah Bern

An atomic force microscope (AFM) is a versatile instrument. It can be used to map out the surface topography of an object with atomic-scale resolution, perform nanomagnetic imaging of the surface and can even manipulate individual atoms. Typically a nano-scale probe is mounted underneath the end of a "spring-board", and a laser is reflected off the top of the cantilever. As the probe traverses the surface, these bumps and holes exert a force on the probe, deflecting the end of the cantilever and changing the path of the laser. In this manner the AFM can "feel out" the surface's contours.

Our project is to design a new, more highly optimized cantilever. Instead of using far-field detection methods, a nano-scale gap between the cantilever and the optical disk would allow for near-field detection. This new configuration would allow the cantilever to be reduced to nano-scale instead of micro-scale dimensions, yielding a high resonant Q factor across a broad bandwidth. In addition, the new configuration would allow the cantilever to be electrostatically actuated should the need arise.

Two Au electrodes, one at given potential and the other at ground, would generate an electric field that the SiN cantilever would experience. The resulting dielectric force on the cantilever would actuate it. The goal is to find the configuration in which the cantilever is most sensitive. We have been modeling two nano-cantilever designs, one with additional Si dielectric under the electrodes and one without. Applying finite element analysis (FEA) to calculate the in-plane dielectric force, preliminary results demonstrate that the magnitude of the force is maximized when one electrode is short and the other tall (for the design without the added Si: -12.3 $\mathrm{pN}\ \mu\mathrm{m}^{-1}$ when one electrode is 270 nm tall and the other is 520 nm, with the cantilever at a displacement of 100 nm from the left electrode, and a separation of 450 nm of the two electrodes). It seems that overall the design without the additional Si is more responsive than that with the additional Si.

Producing any nano-scale device requires a working design and fabrication process, so my work also inolves nanofabrication. In the CNST NanoFab, we have been developing a process that could be used to etch away a Si substrate in a more precise and controlled manner. A promising approach would be to use a backside KOH etching process which would remove that substrate at a specified angle (54.7° to the surface).

This research may allow more sensitive AFM cantilevers to be produced at a reasonable cost and efficiency.

Duke University

Optimizing 3D Structures for the NIST Chemistry WebBook

Michael Liou

Our mission this summer is to enhance the National Institute of Standards and Technology's (NIST) Chemistry WebBook (WB) by performing quality control on its contents and by adding 3-Dimensional (3D) structures. Eight thousand people use the WB on a daily basis; it is a highly-trusted free resource for scientists and students around the world and contains data from many collections, beginning with a boiling point measured in 1813. Currently approximately 114,000 chemical species represented in the WB, but only 27,000 have a verified 3D molecular structure. Our goal this summer is to optimize 15,000 structures and add them to the WB. In addition, we are optimizing 6,000 biochemical molecules from the DrugBank, a pharmaceutical and chemical database, and integrating their chemical information into the WB. Our work is relevant because it diversifies the WB, ensuring its sustainability and credibility for the years to come.

The 3D optimized structures were optimized using Gaussian, a quantum chemistry computer code. Our calculations consist of a series of optimizations, progressing from a simple to a rigorous, time-consuming method. In the first method, a classical (balls and springs) molecular mechanics method (MM2) is applied to give a reasonable starting molecular geometry. The second method is the "semi-empirical" method (PM6), which, unlike MM2, considers electron interactions. Optimizations performed using this method take minutes to optimize and yield a good starting structure from which more complex calculations can be made. The third and most rigorous optimization applies density functional theory (B3LYP) and gives a more accurate and robust optimization. In addition to Cartesian coordinates, the computation returns other useful information such as vibrational frequencies which can be compared to experimental measurements or used as a basis for calculating thermodynamics quantities.

Our other task has been to verify the chemical information that is currently in the WB. Each chemical species has basic identifying information such as one or more names, Chemical Abstract Service (CAS) number, molecular weight, chemical formula, and 2D structure. We confirm that the WB information is correct, and when necessary, suggest changes or corrections. Our work this summer ensures the WB's sustainability and quality, as well as diversifies the overall database.

Optimizing 3D Structures for the NIST Chemistry WebBook

Jennifer Skerritt

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Elon University

Compositional Data Analysis of a Cement Clinker
Amy Zemanick

The production of Standard Reference Materials (SRMs) is one of the measurement services provided by the National Institute of Standards & Technology. This involves measurement to assign values to selected properties of the material, and characterization of the associated measurement uncertainty. SRM 2688 is Portland Cement Clinker with certified values for the mass fractions of the four major phases present (alite, belite, ferrite, and aluminate). The values that were assigned to these fractions are consensus values derived from an inter-laboratory study. This SRM is used by the cement industry to maintain the quality of their products.

Since these mass fractions are parts of a whole (summing to 100 %), they are interrelated above and beyond what the underlying chemistry and mineralogy might dictate. In fact, they are affected by so-called spurious correlations, which generally are negative, because when one fraction increases, at least one other fraction must decrease. Conventional statistical procedures do not take this closure constraint into account. This problem has a long history in the study of the chemical and mineralogical composition of rocks.

In this project, I explored a work-around for the closure problem, to develop estimates of the measurands, and to characterize the associated uncertainties. I used a transformation that John Aitchison proposed in 1982, and that has been widely used since. I compared consensus estimates and associated uncertainties produced by statistical procedures that take this effect into account with those that do not.

Florida A&M University

Digital Multimeter Calibrations
Ronisha Kelley

Why does one calibrate DMM's? The answer to this question is quite simple, but first, answer these questions. Have you ever tried to measure a battery or have you ever gone to buy light bulbs and wondered how the company measured the wattage of the bulb? The answers to these questions are quite simple. DMM's are calibrated to give the proper readings, according to the known standard values, so one may measure such things as battery life, bulb wattage and many more.

In order to get these values, several tests are run on the machine over the different ranges it contains. Although the program to gather the data is already written, the problem lies in the analysis of the data. This summer, the program to analyze this data is to be written using LabView. For each range, there are several values of data, and these values have to be averaged so there is only one value per range. In other words, if there are 10 different ranges, the analyzed data should only contain 10 different values. So far, the program to average the data has been written and verified by test data. However, this is not the end. The analysis also requires looking up a table to find the correction value which corresponds to the gathered data according to its range, frequency, and the units used. This is to correct the offset involved with the calibrator that is used to calibrate the multimeter.

George Washington University

From the Redwood Forest to the Gulf Stream Waters: Creating a Database of Spectral Solar Data Via Locations Spanning the U.S.
Emily Fusco

The US Interagency Ultraviolet Radiation Monitoring Network aims to define short-term and long-term variation in spectral UV-B; to study the variation of UV-B over latitudinal gradients; and to study the effects of clouds and other factors such as aerosols, on UV-B. Over the past 15 years, the Smithsonian Environmental Research Center (SERC) has continuously monitored incident solar UV-B radiation via the SR-18, a multi-channel radiometer that defines narrow wavebands spanning 2 nm wavelengths. Each SR-18 instrument stores a set of raw data, including filter center wavelengths, calibration coefficients, and spectral irradiance values, collected on each day from the calibrated instruments in individual data files. The SR-18 instruments have been operated from various SERC facilities in the US, including Edgewater, MD, Phoenix, AZ, Miami, FL, and Madison, WI. Currently the spectral solar dataset collected from the SERC SR-18 solar radiometers includes 28,000 files of daily UV spectral solar data.

Since the SR-18 data is not accessible to the public, it is necessary to develop a usable database for this data repository, publishing that database, developing a user interface, and preforming analysis on the data. To develop an interactive database, a singular tab-delineated file containing all data is required- the SERC SR-18 data initially received was not available through one file or in a universal format. Following a comprehensive investigation of the different constructions of the 28,000 files, various Java script programs were coded to mine the necessary metadata information from the header lines and bodies of each file, creating a complete dataset. Due to specific record malfunctions, spectral irradiance values for several thousand files were manually computed. By extracting the same metadata from uncorrected data and applying a specifically corresponding correction factor to each individual file, the records were made suitable before adding the information to the overall dataset. Following the standardization of the dataset, it is possible to host the information on a NIST server for the public's convenience and use. A restful API is in development with ELSA and OISM to display a user-friendly web interface to interact with the available data. The interface will allow users to query the spectral solar data for further analysis.

A Study of Polymer Interactions at the Membrane-Solution Interface for Single Molecule DNA Sequencing Applications
Danielle Soberman

Synthetic polymers have many well-known uses in biotechnology (e.g., anti-fouling coatings for biosensors). Recent work at NIST and Columbia University proposed the use of polymeric tags for electronic single-molecule DNA sequencing by synthesis a nanopore (KUMAR, ET AL 2012) . Each of the four tags (which uniquely represent each base) are to be read serially after being released from the target DNA via a single polymerase enzyme attached to the nanopore. The method requires that the capture of the released tags be highly efficient. To study this process, we examined the ability polyethylene glycol (PEG) molecules attached to a lipid headgroup to enter a nanopore embedded in phospholipid bilayer membrane. We also used a Langmuir-Blodgett apparatus to determine the effects of polymer size, polymer surface concentration, and monovalent electrolyte concentration on the surface pressure-area isotherms of mixed lipid monolayers spread at the air-liquid interface. The results demonstrate that the polymer undergoes phase changes that will likely affect its entropy, and therefore its ability to enter the pore.

Georgetown University

Synthesis and Microscopic Characterization of Anisotropic Colloids and Induced Depletion Interactions

George Burton

The purpose of this study is to examine anisotropic interactions in colloidal suspensions and characterize their effect on both the macro-scale rheology and micro-scale colloidal dynamics and aggregation. To do this, we synthesize micron-sized cubic, ellipsoidal and peanut-shaped colloidal particles. These particles serve as a well-controlled model system for understanding directional interactions in more complex systems, such as protein solutions, which are a major focus of the NIST biomanufacturing initiative. In this talk I will discuss the synthesis of these shaped colloids and their characterization with optical, SEM and TEM imaging, and examine the aggregation of these particles due to an induced depletion interaction. Preliminary results characterizing the behavior of these particles under shear using a confocal microscope coupled to a rheometer will also be presented.

Solving Our Carbon Dioxide Problem: Co_2 Binding in Metal-Organic Frameworks

Timothy Dougherty

Metal organic frameworks (MOFs) have shown much promise in a wide range of applications including chemical separations, sensing, catalysis, and gas adsorption. Of major interest, these materials exhibit the ability to adsorb carbon dioxide due in large part to their porous, yet rigid, as well as highly tunable structures. In order to better design MOFs for CO_2 capture a detailed understanding of the precise locations and orientations of CO_2 adsorption sites within the framework structures is required. This study focused on the synthesis and adsorption behavior of the $M_3(BTC)_2$ (HKUST-1) isostructural series (M = Cr, Cu, Mo, Ru; BTC^{3-} = 1,3,5-benzenetricarboxylate). In these materials, metal dimers connect through carboxylate groups to create a local paddle wheel arrangement. Upon removal of solvent water molecules, the activated structure contains a coordinatively unsaturated metal site—a structural element at which binding interactions may occur. The overall structure features a highly symmetric three-dimensional pore system that contains three unique pores: two large channels (11 and 13 Å in diameter) and a smaller tetrahedral-shaped pocket with a diameter of approximately 5 Å. Phase-pure samples of the Cr and Cu analogues were synthesized in gram-scale quantities. Rietveld refinement of neutron powder diffraction data revealed CO_2 adsorption locations at the coordinatively unsaturated metal sites as well as within the small tetrahedral pockets of these structures. Synthesis of the Mo and Ru analogues is ongoing. Future neutron diffraction studies of the Mo and Ru HKUST-1 derivatives will allow for further comparison of CO_2 adsorption within this family of MOFs.

Georgia Institute of Technology

Conceptual Design of a High-Power, Low-Enriched Uranium (LEU) Research Reactor

Max Carlson

At the heart of the NIST Center for Neutron Research (NCNR) is a 20 MW research reactor used to generate neutrons for the multitude of scientific experiments taking place there. While it continues to serve the scientific community, the reactor is nearing the end of its operating license in 2029. Due to the age of the reactor there is a chance the license renewal process will involve significant engineering challenges, and the Operations and Engineering group has shown interest in the consideration of a new reactor design.

To better satisfy the interests of the scientific community, the new reactor should increase cold neutron current and improve the number of instruments able to directly access cold neutrons, while still providing thermal neutrons for specific instruments. The higher current will allow measurements to be completed at a higher level of certainty and in less time. Neutron current, while based on many factors, is proportionally related to reactor power, so a higher-power 50 MW reactor design is considered.

To meet the goals of non-proliferation policies and of the Reduced Enrichment for Research and Test Reactors (RERTR) group, the new reactor should use low-enriched uranium (LEU) fuel. LEU fuel poses a challenge for research reactors since it changes the nature of the neutron distribution inside the reactor in a way that is unfavorable for neutron extraction.

The challenge of a LEU-fueled neutron research reactor was considered, and geometric fuel arrangements that maximize the thermal neutron flux were developed and analyzed. Calculations of various core geometries and expected neutron current performance were carried out using the well-established MCNP5 Monte Carlo particle transport code.

The geometry of a cold neutron source using liquid deuterium was optimized for the specific reactor concept. Finally, fuel cycles, fuel burn-up rates, and thermodynamic concerns (cooling the fuel and the cold neutron source) were addressed using iterative procedures and comparisons to existing research reactors.

Results from the analyses of various effective as well as ineffective conceptual research reactor cores will be summarized. Based on those findings an optimal starting point for further core design considerations will be suggested, along with the expected ultimate gain in neutron current compared to the abilities of the NCNR reactor at present.

Performance Characterization of Precision Positioning Systems

Aidan Clawson

Error budgeting is an engineering management tool to help control and guide the machine design process. It is also a tool to help predict how the final machine design will behave. An error budget allocates resources (allowable amounts of error) among a machine's different components. This is to be done such that the ability of any particular component to meet its error allocation is not exceeded. An error budget is formulated based on connectivity rules that define the behavior of a machine's components and their interfaces, and combinational rules that describe how errors of different types are combined.

To qualify an error budgeting method with regard to systems using linear bearings, we began an effort to conduct measurements analogous to the calculations performed using the method. We performed these measurements on a commercially available linear positioner, and compared them to the values calculated in the error budget.

Gustavus Adolphus College

Characterization and Optimization of Neutron Polarization and Magnetic Field for a Neutron Electric Dipole Experiment

Troy Seberson

The Standard Model of physics is the most complete theory that describes the world around us. However, the Standard Model is known to be incomplete as it omits gravitation and fails to explain dark matter or dark energy which together makes up 95% of the universe. The neutron electric dipole moment (nEDM) may hold the key to understanding these problems in the Standard Model. Current limits put the nEDM as no greater than 2.9x10^{-25} e-cm. Predicted to be non-zero from Super Symmetry and other theories, a discovery of a nEDM would revolutionize our understanding of the universe.

The method to measure the nEDM is being systematically verified through a measurement of the magnetic dipole moment of the neutron (nMDM) which is well-known through previous experiments. Both the nEDM and nMDM experiments use spin polarized neutrons that are reflected many times down a slotted perfect crystal held in a magnetic field. On each reflection a small rotation of the neutron's spin occurs via the interaction with the atomic electric fields in the crystal. The degree of rotation is directly related to the nEDM or nMDM through known physical constants. Multiple reflections in the crystal increases the neutrons' spin rotation to a measurable amount.

Critical to the experiment is maximizing the neutron spin polarization and affirming that the magnetic field is uniform and has the proper direction at each point along the neutron's path. To ensure the neutron's spin is properly oriented at each step within the experiment several experimental components are used to control the spin orientation: a multilayer supermirror, guide field coils, two spin-flippers, and a Heusler crystal. For the maximum number of correctly polarized neutrons, the alignment of the neutron beam with each component was done by rotating and translating each component independent of the others. Analysis of each component's rocking curves allows the optimal location to be known. Complicating things is that many of the components cause unwanted magnetic field gradients that must be minimized. I will present simulations of the magnetic field and neutron polarimetry characterizations for these components.

Hamilton College

Towards Microgram Mass Standards for Small Force Metrology

Brandon Wilson

The primary international standard for mass is currently a physical object, the international prototype kilogram (IPK); however, metrologists are in the process of moving to a standard based on the measurement of fundamental constants. Redefinition of mass is needed since even slight changes in the mass of the IPK result in the need to periodically recalibrate mass standards worldwide. By contrast, defining the kilogram in terms of Planck's constant results in a time-independent definition of mass. This redefinition presents an opportunity to scale the physical principles used to define mass at the kilogram level to much smaller masses with more accuracy than is possible under the current system.

In this talk, I will present a new method for the manufacture of masses below the milligram level using high purity aluminum. Precise mass removal is accomplished through a chemical etch process, while a subsequent electrochemical reaction creates an anodic oxide film that prevents further corrosion and protects the underlying metal. The use of semiautonomous tools for handling small mass artifacts and applications of sub-milligram mass standards will also be discussed.

Harvey Mudd College

Generalizations of Generating Functions for Hypergeometric Orthogonal Polynomials

Michael Baeder

Orthogonal polynomials arise naturally in many problems in applied mathematics and mathematical physics. Generating functions for these orthogonal polynomials are the most important functions associated with them. In this talk, we use connection relations and series rearrangement to generalize generating functions for several orthogonal polynomials in the upper tiers of the Askey scheme whose orthogonality relations are continuous. The Askey scheme constitutes a hierarchy of these polynomials which illustrates how they are connected by various limiting procedures and special parameter values. In our case, connection coefficients express a polynomial as a finite sum of the same polynomial with different parameters. We determine corresponding definite integrals of these generalized generating functions using the orthogonality relations. Furthermore, we derive connection coefficients for some of these orthogonal polynomials, as well as asymptotic expressions and upper bounds in order to complete our proofs.

Hood College

A Preliminary Testbed Architecture Design for the Sustainable Manufacturing Testbed

Alex Paxton

There has been a lack of a unified method for manufacturers and researchers for evaluating the sustainability of manufacturing processes. The Sustainable Manufacturing program has five projects all aimed at developing, using and testing methods of evaluating the sustainability of manufacturing practices. The Testbed for Sustainable Manufacturing project is one of these five projects. The purpose of the initial testbed is to support the testing and development of the sustainability assessment methods and measures that are being developed by the sustainable manufacturing program's other four projects. The testbed is intended for use by manufacturers for evaluating their factories and by researchers for their sustainable manufacturing related research efforts.

The preliminary testbed architecture design currently includes several major components: Modeling Manager, Interpreter, Testbed Configurator, Test Case Configurator, Test Executor, Test Reporter, Service Manager, and System Manager. The Modeling Manager will create a model of a factory. The Interpreter will identify test requirements from user's models and inputs. The Testbed Configurator will be used to configure the testbed components. The Test Case Configurator will be used for setting up test case configuration and support. The Test Executor will run test case within the configured testbed and then, the Test Reporter will analyze the test results and generate test reports for users. The Service Manager will be used for data management, configuration, support, software handling, and general system administration. The System Manager will handle user registration, logging in and out, and project managements.

My work in this project was to help develop the architecture design of the testbed. I did this by developing UML diagrams to help understand the testbed requirements and functions and researching systems integration issues. The UML diagrams I developed include: use-case diagrams, sequence diagrams, and state diagrams, based on system function and requirements. I have investigated APIs and drivers for asynchronous applications. The use-case diagrams explain interactions between users, the testbed, and external input sources. The sequence diagrams describe the order of actions and interactions that occur for each possible activity that the system could engage in. The state diagrams are used to describe the choices and stages which can compose the possible paths that can be taken during program execution.

The talk will cover the UML diagrams I created for the architecture design. It will also include my researching asynchronous input and output, which I created a draft paper based upon.

Software Entropy Sources for Cryptographic Applications
Robert Staples III

Any data encryption method is only as secure as the key that is used in its encoding. Keys are often produced by pseudo-random number generators that use a truly random “seed” value. These seed values must be independent, secure, and rapidly producible. This is where I began my work, studying several methods of random bit generation in an attempt to gain the maximum amount of entropy (or “randomness”).

Computers have a notoriously difficult time being random, due to the fact that they are built with the goal of 100% determinism. There are two main types of entropy sources in computing: hardware sources, and software sources. My work focused solely on software sources, and my testing focus was mainly on a source known as “Clock Skew”.

I studied two promising sources of entropy; developing, testing and tuning each one in an attempt to produce the highest entropy possible. These methods are the intentional thread-race and the harnessing of “clock skew”, or distortion between the system and CPU clocks. Development and informal testing was performed both on a standard Windows desktop and a virtualized Linux environment. I was able to achieve a consistent entropy rate of over 7 bits per byte, almost 88% entropy, in informal testing.

With this research, NIST hopes to gain insight into suitability of software entropy sources.

<u>Indiana University</u>

Friction Effect on Displacement of a Cantilever Beam-Based Instrument During Polymerization Shrinkage
Kwami Lamadokou

The shrinkage that occurs during the composite solidification process (polymerization) is a major stress source for the failure in dental restorative materials. Polymerization stresses (PS) of resin-based dental materials have been measured using a variety of methods. With American Dental Association Health Foundation, NIST has developed a cantilever beam-based instrument to characterize the PS. In this device, composite (or resin) specimens are mechanically attached to a calibrated cantilever beam via a quartz rod adhesively in contact with the specimen, which is also adhesively attached to a fixed lower rod. Tygon tubing is used to encase the rod and testing specimen. With this device, composite polymerization shrinkage stress induces a deflection in the calibrated cantilever beam. The deflection is measured using a capacity sensor. The PS is then evaluated through a beam formula according to the measured deflection. Through finite element analyses, this study focus on the frictional effect between quartz rod and Tygon tubing sleeve on the measurement results.

James Madison University

Characterization of NIST-4 Components and Materials

Eric Leaman

The kilogram is the only SI unit still defined by a physical artifact, the International Prototype Kilogram (IPK). This definition has several shortcomings, including limited access and fear of contamination. Laboratories and researchers around the world are working to redefine the kilogram in terms of the Planck constant. Currently under design is NIST's fourth generation watt balance, NIST-4, which will be optimized to realize mass once the value of *h* has been fixed. NIST-4 is an equal arm beam balance with a coil that hangs from one side. This coil is suspended inside a magnetic field from a stirrup consisting of multiple flexures. The watt balance experiment is composed of two modes: a velocity mode and a force mode. During the velocity mode, the coil is moved through a magnetic field while the velocity and the induced voltage are measured. During the force mode, a current is passed through the now stationary coil and the generated force is compared to the gravitational force on a mass. Alignment of the coil, the magnetic field, and the vertical direction is crucial.

To help minimize uncertainty in NIST-4, components of this new watt balance must be characterized to determine proper materials to use and methods for damping to eliminate parasitic motion. Contributors to measurement uncertainty include vibrations in the coil, the balance support, and in under-damped flexures, as well as any other unwanted motion in any part of the apparatus. In the summer of 2013, some of these components were analyzed to determine the significance of unwanted motion.

An optical measurement stand was built and an experiment was designed to determine both the damping ratio and stiffness of flexures using a simple beam and sliding mass. Accelerometers and piezoelectric actuators were utilized to perform vibrational analysis on the coil. Using both the LabVIEW and Python programming environments, software was created to collect and analyze the data. Based on this work, design recommendations on several crucial NIST-4 components were made.

Johns Hopkins University

Structural Robustness of Reinforced Concrete Frames

Isaiah Sampson

Robustness is the ability of a structure to withstand local damage without widespread failure. This quality has gained heightened awareness since 9/11, where the plane impacts eventually led to the total collapse of the World Trade Center towers. The Structures Group in EL is seeking to develop computer simulations that adequately describe the behavior of damaged structures. A series of full-scale tests on reinforced concrete frames have been performed to evaluate structural performance after local damage. The concrete frames were either cast-in-place or precast, spanning two bays with a stub center column. Vertical displacement was imposed on the center stub column until steel reinforcing bars fractured. The experimental data from these tests will be compared to models created using LS-DYNA finite-element software. The experimental data and validation of the models will support the development of guidelines and standards for design of robust buildings.

Fabry-Perot Displacement Interferometry in Air
Elizabeth Skerritt

The precise and accurate measurement of the SI units is a core mission of NIST. The standardization of the units helps guarantee the uniformity of measurements over time and space. The farad, the SI unit of electrical capacitance, is a key component in electrical metrology and is measured using a calculable capacitor. An important factor in precisely measuring the farad using the calculable capacitor lies on the making absolute displacement measurements.

To make such measurements, interferometry is employed. In the previous calculable capacitor a single beam was used, now we looking to develop a multi-wavelength interferometer which can provide better precision. Previously, it was demonstrated that a Fabry-Perot interferometry could measure displacements of up to 50 mm with a fractional accuracy of 4×10^{-10} in vacuum at 633 nm and 1560 nm. The goal of this project is to extend the approach to displacement measurements in air as well. A well-known approach to compensate for the refractive index of air without relying on independent measurements of the temperature and pressure is to use two wavelengths. We supplement our laser at 1560 nm with an additional laser at 1064 nm in order to control for the dispersion of air where both lasers are working simultaneously. With this setup, we are also able to lock our lasers to an optical frequency comb, which is a powerful tool capable of transferring the radiofrequency domain stability source of cesium clocks onto the wide band of optical frequencies.

In this talk I will cover the theory behind this calculable capacitor and how my research is important in standardizing the farad. I will then discuss how I aided in designing and constructing a fiber laser based interferometer to achieve accurate displacement measurements in air by using LabVIEW and PID controllers to lock lasers of different wavelengths to a Fabry-Perot cavity.

Fourier and Gegenbauer Expansions of a Fundamental Solution of Laplace's Equation on a Hypersphere
Rebekah Wheatley

For a fundamental solution of Laplace's equation on the *R*-radius *d*-dimensional hypersphere, we compute the azimuthal Fourier coefficients in closed form in two and three dimensions, and give an integral representation for the higher dimensions. We also compute the Gegenbauer polynomial expansion for a fundamental solution of Laplace's equation in hyperspherical geometry in geodesic polar coordinates. Furthermore, we show that the Gegenbauer expansion locally matches up to the generating function for Gegenbauer polynomials, which corresponds to a Euclidean fundamental solution of Laplace's equation.

Juniata College

Optimization of Field Flow Fractionation Parameters for Use with Water Soluble Gold Nanoclusters

Avery Fordham

With the increasing use of metallic nanoparticles (NPs) in industrial and commercial products, their sustainability relies on more complete risk assessment in biological and environmental media, including thorough physicochemical characterization of the entire product distributions resulting from processing. The development of analytical techniques capable of detecting, characterizing, and quantifying the broad distribution of products resulting from NP transformation are needed to accurately assess these risks from current and emerging NP-based technologies. Here, we examine the measurement capabilities of hyphenated asymmetric flow field-flow fractionation (A4F) systems for probing sub-5 nm gold and silver species, because a dearth of reliable tools for characterization and quantification of products in this size regime currently exists. We developed synthetic procedures for water-soluble nanoclusters of distinct size (nuclearity) with different ligands to evaluate the selectivity and lower size limits capable of being detected and characterized with the hyphenated A4F-UV/Vis-FLD-DLS-ICP-MS system. By using the pure, ligated nanoclusters as internal calibrants for size-based retention determination under optimized conditions, examination of polydisperse systems, which include plasmonic nanoparticles and ligated nanoclusters, were evaluated to determine the efficacy of the fractionation, characterization and quantification in more complex mixtures.

Rydberg Rubidium Atoms for Charge Exchange in a Penning Trap

William McGrew

A beam of rubidium atoms in Rydberg states is produced for charge exchange experiments aimed at making hydrogen-like ions confined in a Penning trap, which may enable a determination of the Rydberg constant independent of the proton radius. The Rydberg constant is one of the most precisely measured constants of nature. It is determined from the measured frequencies of atomic transitions in low-lying states of hydrogen. The limitation to the accuracy is due to uncertainties in the size of the proton involved in calculating the properties of low angular momentum states. Rydberg states with high angular momentum, on the other hand, are not sensitive to nuclear properties; hence, using hydrogen-like ions in Rydberg states is an interesting possibility. To produce hydrogen-like ions, an atom (such as helium or neon) is first stripped of all its electrons by an electron beam ion trap (EBIT). These bare nuclei are stored in a Penning trap and allowed to interact with Rb atoms in a Rydberg state, taking the valence electron from the Rb atom. The rubidium atoms are produced in an oven, propagating into the Penning trap as a beam at thermal speeds. As it passes through the center of the trap, it interacts with laser beams, which excite it into a Rydberg state. Due to a strong (~3 kG) magnet in the trap, the excitation energy is shifted by the Zeeman effect. Rydberg states are detected by applying an electric field to ionize the excited rubidium atoms; the electrons that are released are collected by a Faraday cup. The Faraday cup signal can be used to characterize the production of Rydberg states.

Kansas State University

Evaluation of a Diamagnetic Levitation Apparatus for Determining AFM Force Calibration Factors and Spring Constants

Brian Blankenau

When studying a material's nanoscale frictional properties with an atomic force microscope (AFM), it is typically necessary to know the force calibration factors for the AFM setup with a high degree of accuracy. While methods for determining both the normal force and lateral force calibration factors do exist, many have significant drawbacks. They either require specialized equipment or are associated with a relatively high degree of uncertainty (greater than ten percent). One newly established technique for straightforwardly determining the lateral force calibration factor with accuracy and precision is the diamagnetic lateral force calibrator (D-LFC) method. The D-LFC apparatus consists of an AFM-compatible sample comprised of a piece of highly-oriented graphite (or "shuttle") that is diamagnetically levitated above an array of alternating permanent magnets. To obtain the lateral force calibration factor, the tip of the AFM cantilever is brought into static contact with the graphite surface as the magnets are swept laterally below. A force is directly calculable from this known displacement and the effective spring constant of the shuttle, which is determined from measurement of its resonance frequency and quality factor in the magnetic field. The calibration factor is then derived from the change in lateral signal recorded during the sweep. We found that the same apparatus may be used as a reference spring for calibrating the cantilever's normal force constant. In this presentation, I will discuss several steps we have taken towards experimentally and theoretically evaluating and improving both of these calibration techniques. I will describe the new method of normal spring constant calibration using the D-LFC and present the dependence of each method on the lateral tip position.

LeMoyne College

Dynamical Structure Measurements of Biotherapeutics with Hydrogen/Deuterium Exchange Mass Spectrometry

Emma D'Ambro

Dr. Hudgens' group is currently conducting research on the dynamical structure of proteins and glycoproteins using hydrogen-deuterium exchange mass spectrometry (HDX-MS). HDX-MS is a method for determining the conformational dynamics of proteins by observing the exchange rates of hydrogen for deuterium along the protein amide backbone. This means that HDX-MS can be used to determine the active configurations of proteins which can be used in many applications, including pharmaceutical drug research.

In the next few years many biological drugs will go off patent. Unlike small molecule drugs such as Lipitor, biological drugs such as Enbrel are large and difficult to replicate as a generic. Our group is part of a larger project that is researching ways to aid the manufacture of generic biological drugs. The goal is to make biological drugs more affordable to those who need them.

We studied a small model protein, bovine ubiquitin (8.5 kDa), which is found in most cells of eukaryotes. With the utilization of a state-of-the-art fully automated HDX-MS instrument, we can obtain 100% sequence coverage information of ubiquitin. The complete sequence information of ubiquitin has allowed us to successfully characterize its conformational dynamics, time-dependent stability, and also the reproducibility of our instrument. We also examined the effects of different denaturants on ubiquitin that provided novel information of the folding-unfolding mechanism of ubiquitin with high spatial resolution. The possible end product of this study is to establish HDX-MS as a method for comparing biological drugs, therefore facilitating the generation of generic biologics.

Bose-Einstein Condensation of Photons
Erin Marshall

Bose-Einstein Condensation, which won Carl Wieman and Eric Cornell the Nobel Prize in Physics in 1995, occurs when a macroscopic fraction of the particles in a sample relax into the lowest energy state. Widespread experimentation has been performed on atomic condensates, but Jan Klaers et al. demonstrated the first ever Bose-Einstein Condensate of photons in 2010.

Photonic Bose-Einstein Condensation is intriguing because BEC is often viewed as a fourth state of matter. While atoms in a BEC experience a thermalization followed by a condensation of their velocity and spatial distributions, photons in a BEC experience a thermalization and a condensation of their transverse mode distribution.

The experimental setup consists of a Fabry-Perot optical cavity, through which light is transmitted, and a medium inside the cavity which absorbs the photons and spontaneously re-emits them into the cavity mode. A variety of approaches were applied in order to construct a working setup that would produce a photon BEC.

In this talk, an overview of the processes underlying the formation of a photon Bose-Einstein Condensate will be given. I will also describe our attempts to create NIST's first photon Bose-Einstein Condensate.

Lehigh University

Microanalysis of Various Materials Deposited by Atomic Layer Deposition

Spin current generation in nanometer-thick platinum and ferromagnetic bilayers have shown many unexpected observations and thus it is a recent area of excitement in physics. These engineered material interfaces are the key to spintronics applications. In order to fully understand the observed spin-related phenomena, we must accurately measure platinum layer thickness and verify the film morphology. Atomic layer deposition (ALD) was used to deposit platinum because it claims to have sub-nanometer thickness control. Samples with Pt thicknesses of 0.5 to 2.0 nm were deposited onto SiN_x substrate. Cross-sections of these samples were examined using a transmission electron microscope. We measured the actual Pt thickness compared to the expected value from the ALD tool and found that the actual values were close to the expected value, however, the layer thickness was not uniform over the area examined. Additionally, we found that the ALD process does not produce atomically smooth Pt layers.

Lock Haven University of Pennsylvania

The Tale of Two Models
Kyle Leber

This project is primarily about enhancing an existing 3D application for human body visualization and measurement using a common web browser. Being able to accurately measure and study scaled three-dimensional models of the human body is a useful tool in many industries. Anthropometry is the science that defines physical measures of a person's size, form, functional capacities, and their interaction with tasks, tools, machines, vehicles, or personal protective equipment. Using web technology such as Javascript, JQuery, and X3DOM, it is possible to visually represent and interact with such data. By combining newer technological capabilities of 3D web, X3DOM, and the dynamic features of Javascript and JQuery, this application enables the user to perform measurements between a wide variety of known anatomical landmarks and can be compared to other models.

Louisiana State University and A&M College

Optimal Photon Down-Conversion Through Thermal Control of Nonlinear Crystals
Chase Brignac

Quantum information applications based on light often require the conversion of photons from one wavelength to another. This can be done using frequency conversion in nonlinear crystals but high efficiency is needed. To achieve efficient conversion of light from a wavelength of 920 nm to 1550 nm with nonlinear crystals requires precise temperature control of the nonlinear crystal and some applications will require a number of temperature controlled crystals. To do this for four channels simultaneously, we have built a system composed of a Printed Circuit Board and an inexpensive microcontroller, an Arduino Uno, with a small monitor screen. We have written custom feedback controller software for the Arduino Uno. We have also designed our own board that controls a piezo driver to stabilize an interferometer and correct for drift over time. These two controllers have the potential to be useful in several future quantum optics experiments.

Massachusetts Institute of Technology

Investigation of the Potential Genotoxicity of Acid-Modified NanoTitania
Meryem Ok

Dentists and orthopedic surgeons frequently utilize titanium based metals as surgical implants because of their beneficial mechanical properties and high bioaffinity. The development of dental resins incorporating surface-modified titanium dioxide nanoparticles (TiO2 NPs) are emerging as potentially new materials for increasing the overall strength, durability and lifespan of the currently available dental resins. It is believed that these surface-modified TiO2 NPs are non-toxic at the molecular and cellular levels, but data to this effect does not currently exist. Isotope-dilution gas chromatography/tandem mass spectrometry (GC/MS/MS) is an effective tool for characterization of the potential interaction of NPs with genomic DNA and was thus used to measure genotoxicity of the TiO2 NPs for this project. Based on preliminary studies indicating that light exposure may enhance NP genotoxicity, repeated trials were performed in both visible light (exposure dose = 1600 mW/cm2) and dark environmental conditions. This project is in collaboration with the American Dental Association.

Miami Dade College

How to Calibrate a Digital DC-MM-Calibrator Effectively
Markus Moser

At the National Institute of Standards and Technology (NIST) the U.S. representation of the volt is based on the Josephson effect, and since January 1, 1990 a new value for the volt is worldwide in effect. To keep this value accurate, industrially used DMM's are required to be re-calibrated by NIST to provide traceability to national standards and confidence to the market place for measurement instruments.

This abstract describes a highly stable voltage-ratio standard build by NIST and the measuring technique used to establish the value of its ratios. This voltage-ratio standard (volt-box) offers discrete ratios from 1:1 to 1000:1. The resolution is typically between 0.1ppm (10^-7) and 0.01ppm (10^-8), depending on the value of resistance and the voltage sent through. By taking a large number of measurements influenced by random error (noise) we are able to calculate the mean of the measurements and so find the true value (the accepted standard value).

Montgomery College

Identifying the Critical Links in a Network
Rehab Al Ammary

We investigated game theoretic approach to network security. Given the topology of a network, we proposed an algorithm to compute the links that are most likely to fail in the presence of an adversary and have implemented the algorithm in Java. In the process, we developed programs from the spanning tree algorithm, the binary search algorithm, and the network flow algorithms.

Error Analysis on OpenHaRT13 Evaluation
Sarab Al Ammary

Handwriting recognition is a research field with many challenges. In particular, Arabic handwriting recognition is difficult due to the highly cursive nature of the Arabic handwriting and its inherent ambiguity due to omission of vowels and diacritics. Additional challenges involve variability among writers as each person has his/her own distinctive writing pattern, diversity in the image qualities from which the handwriting is captured, and varieties in document structures and topics. The NIST 2013 Open Handwriting Recognition and Translation Evaluation (OpenHaRT) assesses the state of the art in Arabic handwriting recognition and translation. My project involves categorizing the types of error that the Arabic recognition systems make. In particular, we look at categorizing the errors by the words' part-of-speech. To this end, our results show that most of the errors are in words categorized as nouns.

Development of an Apparatus to Measure the Optical Properties of Black Carbon Ice Nuclei
Ian Movius

One of the largest uncertainties for climate change models is the lack of understanding of how clouds form and their influence on the radiative loading of the atmosphere. The formation of clouds is dependent on the dispersion of aerosols throughout the atmosphere. Certain aerosols act as ice nuclei

(IN) by interacting with water vapor/droplets through a variety of physical mechanisms (modes). Aerosol particles that serve as IN are characterized typically as being insoluble in water and having a crystalline structure similar to that of ice. Of these particles, black carbon (BC) is currently believed to be the aerosol with the most significant impact on climate change as it absorbs all wavelengths of visible light (aerosol primary effect), however, there are large uncertainties regarding its contribution to cloud formation processes (aerosol secondary effects), which still need to be quantified. One reason attributed to this uncertainty is the lack of understanding as to how BC acts as an IN in multiphase cloud formation processes, with many studies in disagreement. Understanding how BC acts as an IN in multiphase clouds is important because studies have shown that an increase in the number of atmospheric BC IN leads to an increase in the number of smaller-sized cloud ice crystals. At this time, it is unclear why the effect of BC on ice crystal formation processes is different than that of other IN particles. This increase IN concentration and decrease in ice crystal size is believed to both shorten cloud lifetime and reduce rainfall, resulting in changes to local climate pattern.

The focus of this study is to observe both the freezing parameters of the ice crystals that form from black carbon used as an IN and the optical properties of the resulting crystals. An apparatus is currently being developed to study these ice crystals non-intrusively via both a CMOS camera and a technique named the laser-driven thermal reactor. A previous model of the apparatus had been tested to simulate conditions that would allow for heterogeneous ice nucleation, and although successful, further adjustments were needed to be made both to the apparatus itself and the protocol that dictates the experiment.

New and Rapid Methods to Measure Visibility of Bacterial Biofilms

Trinh Nguyen

Dental polymeric composite fillings typically fail within 5-7 years, most commonly due to recurrent tooth decay caused by acid-producing bacterial communities called biofilms. However, the development and commercialization of new antimicrobial materials that resist biofilm formation are hindered by lack of methods to characterize biofilms. Quantification of even basic properties such as overall viability is challenging in biofilms because many cells become inactive (but still viable) in mature biofilms. Traditional CFU (colony-forming unit) assays overcome the problem of inactive cells by providing nutrients that encourage all viable cells to grow, but this technique takes several days, and results can be inaccurate if biofilms are not evenly and thoroughly dispersed into individual cells. Biofilm activity assays take only hours and do not require biofilm dispersal, but they are only sensitive to active cells. We hypothesize that brief exposure to nutrients will activate all inactive biofilm cells and enable activity assays to detect all viable cells within the biofilm.

Therefore, the objective of this project is to develop and demonstrate a modified activity assay to measure overall biofilm viability using Streptococcus mutans (S. mutans), an acid-producing oral bacteria, and compare with the CFU assay. First, the “awakening” concept was successfully demonstrated in suspended (planktonic) cells by replacing spent medium with fresh nutrient broth and measuring overall metabolic activity using a modified tetrazolium-salt assay. Next, biofilm harvesting protocols based on scraping, vortexing, and sonicating are being compared and characterized for the CFU assay. Once harvesting is optimized, the modified MTT assay will be performed for biofilms and compared to CFU measurements. We anticipate that the activity-based viability assay developed in this study will produce results comparable to traditional CFU techniques and can be used to rapidly assess antibacterial activity of novel materials.

Integration of Adaptive Control in Cyber Physical Systems for Enhanced System Performance

Taqiyyah Safi

Cyber Physical Systems (CPS) are hybrid cyber networks interacting with and controlling engineered physical systems. CPS depend upon the synergy of computational and physical components: sensing changes in physical environment, critical-computing and decision making, controlling the physical environment and networking are well grained into every component, and the actions of all the components and systems are carefully orchestrated for robust and optimal performance of the whole system. Such systems are becoming increasingly ubiquitous with applications in diverse domains, such as health care, defense, emergency response, transportation, physical infrastructure.

The environmental conditions surrounding a physical system are not always consistent. In such scenarios, the system controller should be competent enough to adapt to this change in environment to remain in control of the physical system. Adaptive control is a control method used by the controller in which the parameters of the control system are adjusted during the operation of the system as more data become available from the system. Cyber Physical Systems operate under real-time constraint, often with streaming data and are well suited for the implementation of adaptive controls in response to changing physical conditions. In this talk I will address how real-time analytics with real-time data stream can work with adaptive controls to enhance Cyber Physical System operation under varying environmental conditions.

Development of Silver Nanocomposite Model Systems to Test for Environmentally Induced Nanoparticle Release

Nanomaterials have been used intentionally and incidentally since ancient times. In recent decades the use of nanomaterials has been increased due to the novel uses and characteristics these materials possess when they reach the nanoscale. Silver nanoparticles (AgNP), one highly utilized nanomaterial, are well known for the anti-bacterial effect that they possess, and as a result, AgNP has been used in many products such as surface coating, textiles and composites. While there are many benefits associated with AgNP, there has been a growing concern about their impact upon release or disposal into the environment. Therefore, the focus of this research is to determine the potential for the AgNP release from composite materials under different environmental conditions. AgNC were exposed to UV-light and water independently. The AgNC's physical and chemical characteristics were tested using atomic force microscopy (AFM), and X-ray photoelectron spectroscopy (XPS). Release of AgNPs were tested using inductively coupled plasma mass spectrometry (ICP-MS), ultraviolet-visible light spectroscopy (UV-VIS), and Dynamic light scattering (DLS). As current results show, silver is being released when the AgNC is washed using H_2O. However, as per the UV results, the silver release is inconclusive. The UV exposed samples, according to XPS results, show more silver appearing on the surface. This research is vital for future investigations of AgNP release due to the possible harmful effects on the environment and health.

Mount Saint Mary's University

Determination of Aggregate Size Dependence Effect on Soot Particle Packing in a Macroscale Experiment

Lance Dockery

Soot, or black carbon, is produced following incomplete combustion of hydrocarbons and released into the atmosphere, making it the second largest contributor to global climate change after carbon dioxide. The climate change contribution of soot depends upon its optical properties, which are dependent on the soot particle morphology. The goal of this research was to develop an experiment which could model macrosacle particle packing of soot-like particles, allowing better understanding of how nanoscale soot particle packing contributes to optical properties. Monodisperse spherical beads were adhered together into aggregated particles ranging from 1-unit monomers through 12-unit aggregates in random, rigid conformations. Monomer and aggregate packing was measured in cylindrical and spherical chambers of known volume and varying diameters. Particle count and subsequent packing density was determined from the mass of particles within the packing chamber and the volume occupied by the particles. Particle packing scaling was found to follow $0.74\ N^{-1/3}$, where N = the number of monomers in the aggregate, and particles containing $N > 7$ had packing densities of 0.36. The observed scaling correlates to other observed data for collapsed soot aggregates, indicating scaling over six orders of magnitude for the macroscale and microscale particles. Knowledge of nanoscale soot particle packing contributes to a better understanding of the effect of morphology on the optical properties of soot in the atmosphere.

Muhlenberg College

Investigation of Trevisan Extraction Theory and Framework

Andrea Rommal

True random number generators are based on measurements of a physical process that is believed to be random. The actual randomness in those measurements, mapped into a bit string (0's and 1's), depends on the analysis of the physical process and the details of the measurements. This analysis results in a randomness metric called entropy that indicates the maximum number of random bits that can be extracted from the measurement ("input") string. In addition, the input string may not have a uniform distribution and also may have some bias. The extraction of the desired amount of randomness (limited by the entropy), removal of any bias, and production of a new smaller random string with a uniform distribution is accomplished by a process called randomness extraction. One such extractor is defined by Trevisan's construction, with the added feature of being a quantum-secure strong extractor. Recently, Mauerer et al. published a paper outlining the framework for a number of Trevisan-based randomness extractors as well as a Trevisan extractor program that uses the C, C++ and R coding languages. This talk will outline the concept of randomness extractors, how they would be applied to the NIST true random number generation project, and the trials and tribulations of installing, debugging, and running free, unsupported code.

North Carolina State University

Shielding Designs for a Short-Baseline Neutrino Detector: A Monte Carlo Approach

A new experiment to search for a theoretical 4^{th} flavor of neutrino, the sterile neutrino, is planned to be built at the nuclear reactor on campus. This neutrino has been proposed as an answer to the discrepancy between measured and predicted $\bar{\nu}_e$ flux; the so-called "reactor anomaly." If such a neutrino is found, it will be the first particle discovered that is outside the Standard Model of Particle Physics.

One of the obstacles for this experiment is the protection of the detector from interference from neutron, gamma, and muon backgrounds. Using MCNPX, a software package developed at Los Alamos National Labs, we have worked to design and test various shields using input that closely matches the backgrounds we measure at the proposed detector site. Shields were further optimized based on cost, weight, and how well they reduced neutron and gamma backgrounds.

In my talk, I will present more information on the experiment itself, how the software works, the general traits that a good shield should have, and the future of this work.

Molecular Self-Assembly in Water-Alcohol Solutions
Jackson Waller

Some thermodynamic properties of water are not yet understood despite decades of study. For instance, the entropy of water-alcohol solutions is smaller than predicted for an ideal molecular mixture[1]. A possible explanation for this well-known result holds that molecular clusters of alcohol self-assemble within the solution[2,3], though neither the formation nor the structure of these clusters have been explained in detail. A greater understanding of molecular self-assembly in a simple amphiphilic system has theoretical and applicative relevance; for example, it could shed light on biological phenomena such as protein folding and could contribute to improved usage of surfactants in medicine and industry. In this work we investigate this topic using quasi-elastic neutron scattering (QENS) on a 54% methanol-water solution at temperatures between 200 K and 300 K[4]. Applying a partial deuteration technique allows us to determine whether molecular self-assembly occurs within the solution, as well as revealing information about the structure, motions, and lifetimes of the clusters themselves. We propose that methanol clusters take the form of short-lived micelles around the non-polar methyl groups which undergo diffusive motion throughout the solution. We find minimal temperature dependence of the molecular structuring within the temperature range studied. We are in the process of analyzing the temperature dependence of the dynamics in the system. In particular, by comparing the dynamics of the clusters with the single particle dynamics of the water and methanol molecules, we aim to gain a better understanding of the mechanism of cluster formation and destruction.

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Northwestern University

Sustainable Manufacturing Standards Onotology
Sarah Wolff

Attempts to make manufacturing more sustainable can offset many negative impacts of manufacturing processes, increase the efficiency of those processes, and increase the life cycle and quality of products. One way to support the push for sustainable manufacturing is to promote a better understanding of concepts and terminology at the intersection of sustainability and manufacturing domains. Our project is developing an ontology designed to help non-experts in finding and comprehending of the many standards and regulations in this area. An ontology represents knowledge as concepts and the relationships between concepts as a way to categorize and classify terms. This ontology provides a holistic view of sustainable manufacturing requirements and terminology. As part of the effort, I have surveyed and mapped several standards related to sustainable manufacturing into the ontology, such as the PAS 2050:2011, the specification for the assessment of the life cycle greenhouse gas emissions of goods and services. I have identified relevant standards and helped expand the ontology with life cycle, manufacturing processes, and standards concepts and terminology. I have tested and evaluated the visual interface of the software and the import plugin, as well as support the interface extension with additional features. My contribution will be realized in demos of the ontology software created by NIST researchers that could eventually be adopted and utilized in industry or standards-developing organizations. The software and ontology ultimately will aid users in making the decisions to make manufacturing design and processes more sustainable.

Oberlin College

Redefining Acceptable White Light for General Lighting
Mira Fein

Rendering the natural color of an object is an important goal of the lighting industry. In order to achieve this goal, light sources must produce a high quality white light. The chromaticity standards for fluorescent lamps were developed and accepted internationally over thirty years ago by the American National Standards Institute (ANSI). Recently, ANSI also developed a standard for LED lighting products, but it is based on the preexistent fluorescent lamp standards rather than on human color perception data. Recent development in LED technology allows for finer tuning of the light spectra emitted by light bulbs. With the introduction of LED lighting into the general market, color quality issues have resurfaced, leading to the hypothesis that actual preferred white light does not fall within the ranges specified by current standards. If this hypothesis is correct, and current standards do not address perceived white light preferences, a new standard must be developed to address these new technologies. While the color rendering ability of lights can be assessed using various color theories, these assessments do not align with human perception preferences. The key purpose of developing a new standard is to create the most satisfactory lighting for human color vision. To verify this hypothesis and determine visually preferred white light loci, we have conducted a vision experiment including 18 human subjects. Using the NIST Spectrally Tunable Lighting Facility, we have tested a wide array of colors and color temperatures in a natural and familiar setting. Although current standards define acceptable lighting as hovering around the blackbody locus, we predict, and preliminary analysis of our experimental data supports, that actual preferred white points lie significantly below the blackbody locus, outside the ANSI standard range, for a number of color temperatures. The findings of this study can be used as a basis for the development of a new standard that allows manufacturers to produce lighting products that are preferred by people, rather than lighting products that produce unnatural illumination.

Environmental and Economic Sustainability of Residential Buildings
Samuel Sharpe

In the past few decades, experts and political figures have been calling for an energy independent United States to potentially solve numerous political and economic problems, but do not always agree on how it should be accomplished. Should the U.S. increase domestic fossil fuel production? Is alternative energy the way to go, and if so, is it too expensive? The simplest way to solve this debate may be through increased efficiency. This project illustrates that residential buildings can be easily designed to not only be more energy efficient, but also lower costs and positively impact the environment.

This project explores the sustainability (energy efficiency, environmental impacts, and the cost effectiveness) of residential buildings across 4 building code editions for 10 building types (number of floors and floor area) across 229 U.S. cities (9,160 unique cases). We apply energy simulation software to estimate a building's energy consumption. The energy uses are combined with construction and operational cost data to generate a database of Life Cycle Costs and Life Cycle Environmental Impact Assessments.

The results can be utilized to compare costs and emissions across building code editions, locations, and building types to discover the potential environmental and economic benefits and costs of adopting newer editions of the residential IECC code. The implications of this data provide opportunities for supporting investment choices and influencing policy decisions related to residential building codes, technologies, and designs.

Ohio Northern University

Machine Tool Performance Under Loaded Conditions
Kathryn Skobrak

The need for smaller tolerances on machined parts is becoming more pressing as the complexity of parts increases. Machine tools are machines that make parts; with tighter part tolerances, machine tools need to become more accurate. One step towards reaching this goal is to evaluate the performance of the machine in order to understand the errors of the produced parts, and then be able to compensate for those errors. Currently, the international standards for machine tool performance only cover testing under no-load conditions. Measurements are taken when there is no force between the tool and the workpiece; that is, while no piece is being machined. A devise and method are being developed to evaluate the performance of a machine tool under loaded conditions, with a tool-workpiece force and no machining during the test. The design uses pneumatic actuators to apply variable vertical, lateral, and longitudinal forces between the tool and workpiece. Research was done on instrumentation design and assembly, data acquisition setup, test calibration, and performance data under loaded conditions. The strain gage network was designed and the network was assembled for the vertical force tests, fixtures were designed for existing laser metrology equipment for use during testing, and testing scope was determined based on International Standards for no-load machine tool performance. Preliminary tests were performed on a vertical machining center and the data was analyzed to yield the machine stiffness and errors as a function of load.

Oklahoma State University

Solution Chemistry and Kinetics of High Volume Fly Ash Binders

John Seader

Sustainability of the U.S. civil infrastructure depends, in part, on the assured use of higher volumes of fly ash in concrete binders than is currently allowed in building codes. Using higher volumes of fly ash reliably will require and better understanding of the chemical and structural changes that occur in such binders at early times, that is, the changes that determine the setting time of concrete. This project involves the systematic chemical characterization of the aqueous solution in high volume fly ash binders at early times using inductively coupled plasma optical emission spectroscopy (ICP-OES) and simultaneous tracking of the chemical reaction rates using isothermal conduction calorimetry.

Princeton University

Automating Image Edge Detection with Accuracy Comparable to Manual Reference and Correlating Oct4 GFP Gene Reporter Expression with Antibody Label for Oct4 in Stem Cell Colonies

Catherine Breen

The method of gradient thresholding, taking the gradient of pixel values and selecting a specific value in which exceeding values pertain to the edge, results in edge detection. Biologists and cell analysts need an automatic method for edge detection for segmentation of cell colonies, yet current techniques are not sufficiently robust to handle the most commonly used image channel from a microscope, phase contrast, and are inconsistent in their segmentations. This study compares how the intensity gradient mean, median, and mode segment an image to the ideal segmentation created by manually finding the best threshold of the gradient image. The images are in phase contrast modality and three different cell lines are studied for this analysis: (1) Stem cell colonies, (2) NIH 3t3 cells, and (3) Sheets of breast cancer cells. Dice metric is used to evaluate the similarity between images segmented using the manual threshold (reference image) and the automated one, using the mean, mode, or median of the gradient. A potential correlation relationship between these values and the manual threshold is found where Sobel and Prewitt gradient showed a consistent relation between (mean, median and cell density) and the manual threshold. The average similarity between all these images using Dice is 0.8. This proves that the automated segmentation is performing well when compared to manual segmentation.

The GFP protein exhibits green fluorescence when excited by blue light, making it a convenient reporter label for biologists to identify the activity of genes. In order to use the GFP signal as a gene reporter, it is important to understand the relationship between the expression of GFP in cells, and the actual presence of the protein for which GFP serves as a reporter, by an orthogonal measure such as antibody labeling in cells. By analyzing GFP expression in live cell cultures and antibody label for Oct4 in the same cultures, this study will assess correlation between the two.

Purdue University

Standard Reference Mortar Development
John Epling

The primary goal is to develop a reliable and consistent method to calibrate conventional concrete rheometers. Typically standard reference oils would be used to develop a standard calibration for these machines to account for zeroing and slippage errors. However, since concrete, specifically for this project mortar, contains suspended aggregates this technique would not accurately reproduce reliable measurements from current concrete rheometers. Consequently, NIST developed a standard reference material (SRM) for paste or SRM 2492. After obtaining a new rheometer for the engineering laboratory, the first step was to calibrate the new device using the SRM 2492 and standards oils regarding traditional geometries such as parallel plates and coaxial. Throughout these test several issues were uncovered and resolved regarding the calibration methods. The main goal this summer was to develop an SRM for mortar. In order to simulate mortar, 1 millimeter diameter glass beads where added to SRM 2492 at different volume percentages. The mixtures were then tested using a number of rheological geometries, including coaxial, 4-vane, and 6-vane tools. Overall, this approach has proven to correctly characterize mortar. Definitive data will be presented for each stage of this SRM mortar. Eventually, the development of this SRM mortar will be used to create a standard reference concrete for rheological experimentation using larger glass beads.

Reed College

Reactor Data at Your Desk
Isaac Khader

The NIST Center for Neutron Research houses a 20MW nuclear reactor, which first reached criticality in 1967. While the reactor and the NCNR facilities have experienced numerous upgrades over the years, much of the control room has remained the same. This means that a significant amount of the reactor data such as valve states and water temperatures were until recently only viewable on the control room console via analog indications. While operators seated at the control console did have access to a few digital indications and historical data for some parameters, there is no way to access any of the data remotely.

Recently an OPC server and a PC configured with LabVIEW have been set up to consolidate reactor data into a database. That computer pushes the data from all of the control room through a secure firewall onto the NIST network. The present value data is stored on a virtual server in a MySQL database.

This project involved designing a graphical interface to display this data from reactor systems in a useful manner. This was accomplished with two main features: display of current reactor data on mimics of relevant systems, and charting of historical data. A C#.Net program was created to implement these features. It can be installed on any NCNR computer. This program queries the MySQL database to obtain current and historical data.

In order to make the data accessible on portable devices such as iPads or if the user does not have access to the C# version, an Apache web server was set up on the virtual server with the present value database. This Apache web server hosts an internal web page with an index that allows the user to select current data on the mimics.

Rensselaer Polytechnic Institute

Thermal Processing Impacts on Slow Growth
Resistance of High Density Polyethylene
Whitney Novotny

Polyethylene pipes are used extensively across the world for gas and water distribution due to their resistance to corrosion, relatively low cost, and lower failure rate compared to metallic and concrete piping materials. In gas and water pipeline applications, heat fusion joining (also called butt welding) is one of the preferred methods of joining polyethylene pipes and fittings. Heat fusion involves melting the pipe and/or fitting ends and pushing them together to create a joint. This method has been used for decades to successfully weld sections of pipe. However, fusing is a complicated thermal process that requires melting the material and diffusion of polyethylene across the interface to create the bond between the pipes. Recently, the Nuclear Regulatory Commission has shown that fusion joints may be more susceptible to slow crack growth failure compared to the parent pipe material.

The current phase of this research focuses only on the thermal processing step. Unimodal and bimodal polyethylene resins were subjected to the thermal treatment (temperature and pressure) in the ASME Boiler and Pressure Vessel (BPV) codes that govern thermal fusing for high-density polyethylene (HDPE) used in safety applications for nuclear power plants. The resistance of the resin to slow crack growth after processing was measured using a novel strain hardening method identified in the literature. The impact of thermal processing on crystallinity within the resin was measured through dynamic scanning calorimetry (DSC). Finally, the impact of thermal processing on the local creep behavior was measured through nanoindentation.

Rochester Institute of Technology

Evaluation of Thiolacetates and Disulfides as Lipidic Anchors
In Tethered Bilayer Membranes (tBLMs)
Perri Weinstein

Integral membrane proteins (IMPs) are essential for communication between cells and their environment. These proteins include a wide variety of functions - channels such as the K^+ and Na^+ channels, receptors such as the G-protein-coupled receptors (GPCRs), and enzymes such as glycosidases. Tethered bilayer lipid membranes (tBLMs) create a lipid bilayer environment adjacent to a surface for studying IMPs, which are generally more difficult to sustain their native structure than soluble proteins. Previously, the anchoring of the tBLMs to the substrate (Au) was accomplished using tether molecules terminating in a thiol (-SH) group. However, thiols exhibit limited storage; reacting oxidatively resulting in the formation of disulfides that seemed to affect the reproducibility and quality of tBLM formation. The tether molecules thus required constant monitoring of material purity and cleanup. These issues could be solved with the use of tethers terminating in thiolacetates or disulfides, which are more stable.

My research consisted of material preparation, analysis, purification, and assorted surface science measurements on thiolacetate and disulfide self-assembled monolayers (SAMs) and tBLMs. Mixed SAMs were formed on the surface of a gold substrate using either the thiolacetate or disulfide derivatives of the previously prepared lipidic anchor thiol WC14 [WC14 = $(CH_2CH_2O)_6CH_2CH(OR)CH_2(OR)$, where R=$C_{14}H_{29}$] and 2-hydroxyethane disulfide (the disulfide of β-mercaptoethanol) or the thiolacetate of the methyl ether of β-mercaptoethanol ($CH_3COSCH_2CH_2OCH_3$). Synthesized materials were analyzed by thin layer chromatography and nuclear magnetic resonance spectroscopy. Spectroscopic ellipsometry was used to measure the growth of the thiolacetate and disulfide SAMs, with comparison to the literature data of WC14, while contact angle and neutron reflectometry were used to characterize the orientation and composition of the organic film. Finally, electrochemical impedance spectroscopy was used to measure film capacitance, which determines the completeness of the SAMs/tBLMs.

Overall, this summer has been very crucial for future research on tBLMs. Mixed SAMs made with thiolacetates or disulfides hold promising results that will be discussed throughout my talk.

Rowan University

Measurement of Magnetic Anisotropy in Magnetic Nanoparticles

Christopher Kassner

Magnetic nanoparticles have been found to have a major impact on modern technology, especially in biomedicine. New methods of drug delivery, cancer treatment, and imaging have been developed through utilization of magnetic nanoparticles. Magnetic nanoparticles have been used to nearly completely regress severe mammary tumors in mice through active magnetic nanoparticle hyperthermia treatment. They have also been used to develop a new imaging technique called Magnetic Particle Imagining. In particular, in magnetic nanoparticle applications, the magnetic anisotropy has been shown to be a controlling parameter, determining the effectiveness of a given magnetic nanoparticle system for the application. Herein, we used a Vibrating Sample Magnetometer (VSM) to determine the anisotropy of iron-nickel zinc ferrite nanocomposites as a function of the heat treatment temperature. Similar measurements were also performed on cobalt nanoparticle systems suspended in dichlorobenzene. The samples were cooled to temperatures ranging from 150 to 200 Kelvin during the measurement. A series of torque measurements were performed and analyzed to determent the anisotropy coefficients (Uniaxial K_U and Unidirectional K_D) for each nanoparticle system. We found that the uniaxial component decreased monotonically with increasing annealing time. However, the unidirectional component decreased with annealing, but varied with annealing temperature. This coincides with a change in the composition through oxidation of the iron nanoclusters. Therefore, these results demonstrate the complex interrelation between magnetic anisotropy and composition.

Improved Data Comparison Schemes for Inter-Laboratory Studies on High-Pressure Gas Sorption Data

Troy Smith

Nanoporous materials are being studied for commercial and industrial applications, including fuel storage, CO_2 gas separation, catalysis, environmental remediation, and gas purification. The number of available nanoporous materials continues to grow, with new material types, such as metal-organic frameworks (MOFs) joining the traditional adsorbents such as zeolites and activated carbons. Determining the sorption properties of these materials is critical for designing materials with improved characteristics according to the intended application. However, achieving reproducibility in high-pressure sorption measurements is a challenge itself, due to the lack of universally accepted standards and testing procedures for adsorbent testing. This makes the comparison of data between laboratories a formidable task, and for this reason, the high-pressure gas sorption community would benefit from having improved data comparison schemes. In this work, a curve fitting tool for modeling high-pressure gas sorption isotherms was developed in order to fit experimental data points to continuous functions. With these functions, many data points can be reduced down to three or four model parameters that can be further analyzed, without having to compare entire isotherms and their associated data points. Just as well, comparisons to other data sets are simplified since the data is fit to a continuous function (gas uptake as a function of pressure), which allows any pressure or gas sorption uptake to be compared instead of individual experimental points. From these function parameters, we can also generate isosteres and find the isosteric heat of adsorption, using another tool designed in this work. We have applied this methodology to high pressure CO_2 and N_2 sorption data on two common porous materials (zeolite 5A and ZIF-8) from a pilot-scale inter-laboratory study initiated between NIST and the University of Sydney, Australia. Based on results obtained, several data comparison indicators are proposed and discussed.

Rutgers University

Optical Ferromagnetic Resonance Measurement Using the Kerr Effect
Katherine Sytwu

Magnets are a significant part of modern technology, providing electrical generation and transmission, information storage, medical imaging, entertainment, and more. Most of the magnets we use in daily life are ferromagnetic materials, which can be magnetized and potentially contain complicated magnetic domains. Since magnetic materials are used in a wide variety of applications from macroscopic to nanoscale, it's important to have fast and accurate characterization tools. One such tool is ferromagnetic resonance (FMR). In FMR, magnetization rings at gigahertz frequencies and the resonance frequency carries information about the magnetic properties of the material. Typically, FMR is detected inductively through contact with a waveguide. Non-contact optical techniques, however, are advantageous as they can be done from a distance and aren't limited by the frequency range of a waveguide. Current all-optical methods use two laser beams, a pump and a probe, to separately drive and measure FMR using the Magneto Optical Kerr Effect (MOKE). We simplify this setup by combining the pump and the probe into one modulated laser beam that simultaneously drives and measures the dynamic Kerr effect. This method streamlines the detection process and allows for future work in observing multiple resonances with one measurement. In this talk, I will discuss the principles behind FMR and MOKE, and the process behind setting up a dynamic Kerr measurement.

Savannah State University

Measurement Science for Concrete Surface Electrical Resistivity Test Methods
Sterling Brooks

NIST is working through ASTM International to standardize a new test method for the electrical resistivity of concrete cylinders using the Wenner 4-electrode surface measurement technique. A standardized test procedure will help to insure that anyone performing the measurement can achieve a consistent level of repeatability. Furthermore, the process needs to be applicable to varying cylinder sizes, and to both cast and cored concrete cylinders. Because a number of concrete performance properties (diffusivity, sorptivity, corrosion rate) are related to resistivity, this standard test method could be utilized for performance assessment. In addition, the electrical conductivity can vary with changes in the concrete mixture design and in changes in the construction processes, so it may also be a useful means of monitoring consistency throughout construction. The reliability of the test method was improved by studying the required number of measurements, and whether measurements made on cored cylinders required any modifications to the measurement process established for cast cylinders. The current process of repeating four measurements around the outside of the cylinder was sufficient to achieve a suitable number of measurements and to overcome spurious variations due to heterogeneities. Measurements made on cored cylinders indicated that, for the type of large aggregate used, the measurement reading is not sensitive to the precise location of the surface electrodes.

Automation of Performance Plan Generation
Leticia Simpore

At NIST (National Institution of Standard and Technology), employees must submit a written accomplishment performance plan to their supervisors. This performance plan must meet some expectations according to the employee position level. Supervisors, based on some critical elements, will evaluate the employee’s performances. Employees failing to meet these expectations may be disciplined, reassigned, reduced in grade or pay band, or removed from the Federal service. It takes a lot of time for employees to put together these performance plans, so it was my job to automate the process as much as possible to minimize the workload on the employee. I am doing this by writing a program that will help to automate the development of the employee’s performance plan. The program should contain the information that is required by NIST policy and is relevant to the employee’s research position. This template is to provide general guidelines to allow the uniformity among performance plans of non-supervisory ZP research staff within EL. The program will be based on the employee’s response to a series of questions that the system will generate. Based on these responses, aspects of the performance plan will be filled out automatically. The VBA (Visual Basic for Application) language, which is a simple programming language that can be used within Excel to develop macros and complex programs, was used to perform this task.

Smith College

Measuring Optical Apertures for Solar Irradiance Monitoring
Sara Stoudt

The Total Irradiance Monitor (TIM) is an instrument on-board the SORCE satellite that was launched in 2003. The TIM measures the total solar irradiance (about 1.4 kilowatt per square meter) incident on the top of the Earth's atmosphere. These measurements play a key role in determining an accurate energy budget for the Earth's atmosphere and to characterize the components of climate change that are unrelated to changes in the "solar constant".

One of the contributors to measurement uncertainty of the solar irradiance is the area of an opening (“aperture”) that collects solar radiation for measurement by the TIM. NIST scientists from the Sensor Science Division have been measuring the areas of these apertures based on the locations of points along the edge of the aperture, determined using non-contact, optical methods. For those apertures that are circular, NIST fits circles to these points by a least-squares method, and estimates the area of the aperture by the area of the best-fitting circle.

In my SURF project I compared the performance of alternative methods for fitting circles to such sets of points and evaluated the influence of the procedure used to sample the points. Based on this comparison and evaluation, I developed recommendations for how to reduce measurement uncertainty, including the adoption of best sampling strategies for the edge of an aperture and selection of best methods to fit circles to them.

Face Recognition Performance in Point-and-Shoot Video
Dana Udwin

Face recognition technology is useful in a world where personal electronics proliferate and the videos you upload need tagging. Such technology is also a boon to security operations when surveillance footage may be informative. How can we maximize the rate of correct classification while keeping the rate of incorrect classification at a minimum? What video qualities have import in achieving this balance?

I analyzed the open-source algorithm Local Region PCA (LRPCA), developed by NIST and Colorado State University, and the commercial algorithm PittPatt. The algorithms ran on the same set of 2,742 videos (filmed across six locations using six different sensors and 265 participants). Although each algorithm generated a similarity score for every frame of every video against every frame of every other video, I looked at the two frames for each video pairing that yielded the greatest LRPCA score and the two frames for each pairing that yielded the greatest PittPatt score.

From there, I looked at the correlation between similarity score and a variety of covariates that describe each frame, such as side-to-side head rotation, face size, head tilt towards either shoulder, setting and camera used. Environment in which a video is recorded (indoors versus outdoors) and activity performed appear to influence both algorithms' success. Determining the respective strengths and weaknesses of LRPCA and PittPatt exposes areas of opportunity for evolution in face recognition technology.

Southern University A&M College

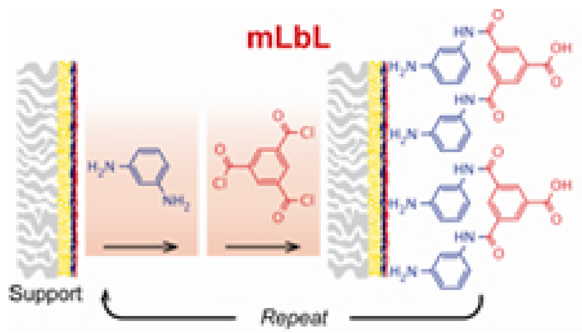
Chemical Structure – Performance Relationships of Molecular Layer-by-Layer Water Desalination Membranes
Shannon Jones-Butts

Access to clean, safe and affordable water is vital to public health, economic growth and national security. Thin film composite (TFC) membranes, having an extremely thin but effective polymer film as the separating layer, are the leading materials for screening the tiniest solutes from water. In order to drive down energy costs for operating such membrane plants, thinner and more efficient membranes are needed.

Current commercial membranes for removing salt from seawater are made *via* interfacial polymerization, where monomer A (a diamine dissolved in water) reacts instantaneously with monomer B (a triacid chloride dissolved in an organic solvent) at the interface between the two immiscible fluids. These monomers react to form a highly crosslinked, dense *aromatic polyamide* film that can separate dissolved ions from water.

In this project, we instead use a layer-by-layer approach to fabricate the separating layer, where monomer A and monomer B are sequentially and repeated reacted on a surface to form the 'active' layer. This layer-by-layer approach opens the door to new monomer chemistries as well as reduces mass-transport limitations inherent to the interfacial polymerization process.

We created 'active' layers made from the reaction of trimesoyl chloride (monomer A) with a variety of diamines and a triamine (monomer B), in an effort to explore the role of monomer structure on the ability of the membrane to remove salt from water. We found that there is indeed a striking dependence of the TFC membrane performance on the monomer structure and functionality, and that much thinner 'active' layers formed via molecular layer-by-layer deposition can still filter out 99+% of salt ions from water!



__State University of New York Albany__

Photoresist Surface Modification for Photolithography
Michael Briggs

Nanoscale manufacturing uses processes such as photolithography, deposition, wet etching, dry etching and many more. While some of these processes are much easier than others, almost every method involves the application of a photosensitive chemical on a substrate that is exposed to light of a certain wavelength, developed and then manipulated using one of the different deposition or etch processes. Etch selectivity and removal post-processing can also be very material dependent.

In my talk, I will discuss two new NanoFab tools used for surface modification in the photolithography process. The first project involved a wideband UV Exposure system which is used for UV curing. Photosensitive chemicals, or photoresists, can be exposed to UV light and heated at 90 C simultaneously as a method of strengthening the resist, making it harder to remove during the etch processes. This method is preferred to the well-practiced post-develop bake step because UV cured photoresists can be removed much easier than hard-baked resists.

The second tool is an oven primarily used for Hexamethyldisilazane (HDMS) vapor priming. This tool recently had an ammonium gas line installed so users can perform image reversal processes as well. Image reversal is the process in which a positive tone photoresist is placed in an ammonia environment which changes the tone of that resist from positive to negative. Depending on process parameters such as pressure, temperature, process time and cycle time, the sidewall angles can change allowing for easier lift-off of deposited metal layers.

My role this summer was to make sure these tools are working properly, to establish Standard Operating Procedures [SOPs] and to develop baseline process parameters for users so they are able to perform these useful processes on their own in the NanoFab.

Probe-Assisted Doping and the World's Smallest QR Code
Chase Brisbois

Moore's Law pushes the limit of conventional technology in order to fabricate smaller devices. Semiconductor doping has been accomplished predominantly with traditional ion implantation. However, as devices scale down in the lateral dimensions, dopant implantation becomes increasingly susceptible to statistical variation from the ion source. Additionally, reducing implantation depth becomes more difficult due to energetic limitations. As a result, it is desirable in the semiconductor industry to create highly local and ultra-shallow regions of doped silicon. To this end, a new technique is being investigated called "probe-assisted doping." This project attempts to introduce boron into Si(111) by coating the wafer with a boron-containing compound (3,4-dimethylphenylboronic acid and 4-vinylphenylboronic acid) and physically push the atoms into the silicon surface using a scanning probe microscope tip. Wafer coating methods will be investigated along with appropriate cleaning and annealing conditions. Using this technique, we will attempt to create the world's smallest QR code by selectively doping a 16x16 "bit" area of silicon. This technology may enable the development of advanced devices for future research or, more practically, novel micro-tagging systems. More complex architectures could be fabricated by employing the use of multiple tips.

State University of New York Binghamton

Optical Measurements of Porosity in Additive Manufactured Metallic Parts
Jessica Gladstone

Additive Manufacturing (AM), more commonly known as "3D Printing", is a relatively new and revolutionary way to build complex geometric shapes using very thin layers (on the micrometer scale). There are many speculations regarding the fields that AM will impact, but most scientists and engineers agree that this technology can greatly benefit the military, aerospace, and biomedical fields. For products like biomedical implants, the measurement of their percent porosity is essential to their implementation. For instance, effective tissue growth in implants requires a specific degree of porosity to ensure that the tissue is properly attached to the part.

One of the most common methods of measuring porosity is taking optical micrographs of the part and performing image analysis to detect pores. Disk samples of known porosity were each cut in half, to expose their cross section. Images were then taken of each cross section and evaluated under a newly generated MATLAB program to determine their respective percent porosity. To reduce the effect etching had on the porosity measurements, a moving average filter was applied to each image.

Although the method requires no additional training to perform, the results of the porosity measurements are quite inaccurate. The desired filter to indicate pores in these images are dependent on many factors, such as surface roughness, pore size, and lighting; therefore, it is difficult, if not, impossible to automate given the parameters of the technique. The images taken are only at the cross section, not the entire sample; therefore, the porosity determined by the program is not an accurate representation of the full sample. In addition, the program is extremely subjective to the user's inputs, so it has been proven to not be as effective in determining percent porosity as desired.

Designing a 100TΩ Standard Resistor
Edward O'Brien

The primary goal of this research is to develop a 100 TΩ transfer standard which can be used as a transfer standard to measure and calibrate other resistors and build-up to 100 TΩ from 1TΩ and 10 TΩ. The 10 TΩ resistor elements were measured, with two different measurement systems, and there correction was found in parts per 10^{-6}. The two measurement systems were a RC charged based system and a modified Wheatstone bridge. Measurements were taken before and after cleaning the resistor elements using acetone and ethyl alcohol in an ultra-sonic cleaner. The twelve resistor elements with the lowest standard deviation in parts per 10^{-6} were chosen and were re-measured to ensure the most accuracy for the transfer standard. Stability and short-term time dependence were considered to select 10 of the 12 resistor elements for the transfer standard. At this high level of resistance there can be many complications since measurements can take many hours and there can be leakage from the resistance element to ground. To reduce this leakage, guard resistor elements of 100 GΩ were then measured which will be used for leakage suppression between the 10 TΩ elements and ground. An enclosure will be built which will protect the circuit, prevent humidity changes, and prevent any radio frequency interference with the 100 TΩ transfer standard, thus minimizing any changes in its value.

High-Speed RF Spectrum Analysis on a Software-Defined Radio
Paul Watrobski

Because of the increasingly limited availability of radio frequency (RF) spectrum, a new form of spectrum access must be developed to utilize the spectrum more efficiently. One possible method for increasing the efficiency is called dynamic spectrum access (DSA). The idea of DSA is to dynamically identify and utilize idle portions of the spectrum while avoiding destructive interference with the licensed user (also known as the primary user). With a testbed of universal software radio peripherals (USRPs), which are software-defined radios, it is possible to develop and experiment with new protocols for dynamic access in realistic RF environments. There are several ways to approach the development of DSA digital signal processing (DSP) with these USRPs: the GNU Radio toolkit, MATLAB Simulink, or the Xilinx Integrated Software Environment (ISE). Developing with Xilinx ISE presents a unique opportunity making it possible to program the USRP's field programmable gate array (FPGA) to handle a substantial portion of the DSP up front, passing more refined data back to MATLAB Simulink for further processing. An FPGA is a versatile tool that allows for inexpensive on-the-fly hardware development. This particular study explores the FPGA option in developing spectrum-sensing functionality within the USRP. With the addition of a fast Fourier transform (FFT) and a Blackman-Harris window, it appears that it may be possible to effectively determine which bands are active or not with shorter latency than on a general-purpose processor. The next task is to develop an RF spectrum detector and to compare it with the above methods to determine which one yields the best results, quality being dependent on the system's speed and accuracy. The best system will be able to make these detections accurately and quickly so as to avoid much or any destructive interference with the primary user's signal.

Massively Parallel Long Term Reliability System
Andrew Wong

Transistors are the fundamental building blocks of electronics today. They are found everywhere and play an important role in people's daily lives. Transistors are implemented in the operation of cars, flights, space shuttles, and life support machines. Indeed, the reliability of these transistors during their expected lifetime is of vital importance.

Because of its superior performance, Metal-Oxide-Semiconductor Field-Effect Transistor (MOSFET) is the most commonly used type of transistors in today's electronics. However, MOSFETs can suffer from several wear out mechanisms that affect their reliable operation.

Negative bias temperature instability (NBTI) in pMOSFET and PBTI in nMOSFET are degradation mechanisms that can result in build-up of defects in the oxide's bulk and creation of traps at its interface. This adversely affects the threshold voltage, the charge mobility, drain current and transconductance of the MOSFETs.

In order to project the impact of this mechanism on the operation and lifetime of the device, accelerated N/PBTI tests are performed to generate and inspect the degradations within reasonable timeframes and high statistical accuracy. During the test the gate is biased at levels higher than the operating range, at an elevated temperature (up to 200°C) while the current is periodically measured to monitor the device parameters shift.

This research project involves the design and implementation of an embedded system that can perform massively paralleled N/PBTI tests including hundreds to thousands of transistors simultaneously. The system consists of a printed circuit board for signal conditioning/monitoring and a software application for high speed data acquisition. The setup will allow the understanding of some fundamental degradation features and help determine their correlation with the device lifetime.

Laboratory Instrument Driver for Home Area Energy Network

Daniel Wong

Smart Grid is a revolutionary concept that will provide a sustainable energy grid system. This modernized system will "enable bidirectional flow of energy," and "use two-way communication and control capabilities," in order to connect micro-generation systems (such as solar cells, wind turbines, and battery storage) to the electric grid. For example, consumers will be able to use energy prices are lower, while selling excess energy from solar cells on their roofs during peak prices. Similar to how our computers and phones are connected over the internet, the Home Area Energy Network (HAN) will allow devices such as HVAC systems, major appliances, home Energy Management Systems (EMS), lighting, and smart meters to communicate information and allow the consumer to better understand and manage energy use.

The goals of the project are to configure a hardware interface that connects the HAN emulator to the laboratory instrument control computer, to characterize the EMS, microgrid Power Conditioning System (PCS), programmable load, and AC source in order to simulate smart grid test scenarios, and to develop a graphical user interface (GUI) and software driver using National Instruments LabWindows/CVI. The GUI configures and initializes the HAN emulator devices from the control computer. In this project, the HAN emulator consists of the EMS, PCS, and the programmable load. The HAN emulator also includes a DC power supply to simulate a photovoltaic cell to test how the system responds to the intermittent nature of solar power. Battery storage is also connected to the HAN emulator to test power cycling and ensuring uninterrupted power to the system. The AC source is connected to the HAN emulator to simulate flow of energy from the energy grid.

State University of New York Stony Brook

Fuzzy Fiber Fillers: Understanding the Metrology and Aquatic Durability of the Next Generation of Polymeric Nanocomposites
James Ging

Epoxies are used industrially as structural composites, coatings, and adhesives. Recent developments show that the next generation of carbon nanotubes (CNT)/epoxy composite may lie in fuzzy fibers, or micro-fiber reinforcement with nanotubes grown axially on their surface. The addition of nanotubes has been shown to increase conductivity and improve toughness to fracture in these brittle systems. These materials have shown potential in structural, health monitoring, and commercial applications as well as the potential to make, tougher fiber composites with controllable conductivity. With their novelty, however, comes the need for a reliable method of determining their composition, mechanical and chemical properties, and their long-term environmental durability.

This presentation will discuss the development of an optimized method for creating CNT/fiber reinforced epoxy composites and evaluating their initial thermal and mechanical properties. Two different levels of CNT growth were used to determine the impact of CNT on mechanical properties. Since hydrothermal degradation of the epoxy-fiber interface is the weak link for long term performance, the composites were exposed water submersion at elevated temperatures (50 C). The water uptake into the composite as a function of time was tracked against the change in mechanical and chemical properties as a function of time. This paper will provide an introduction to these materials and an overview of their long term behavior in water.

Swarthmore College

Extrinsic Lidar Calibration for Use with Mobile Robotics
Justin Cosentino

In mobile robotics two-dimensional laser range are essential for various robot navigation tasks such as simultaneous localization and mapping. These sensors finders (lidars) allow for real time range measurements across large angular fields. However, in order to effectively use data from any number of lidars it is necessary to know each range finder's position and orientation relative to one another and to a world coordinate system.

We propose a method for identifying the rigid transformation between two SICK LMS 200 lidars, allowing for the extrinsic calibration of said coordinate systems. Utilizing a winged target specifically designed to reveal a lidar’s full six degrees of freedom (6DoF) pose, numerous scans are taken from each lidar and a recursive split-merge line extraction algorithm is used to determine the location of the target relative to each lidar’s coordinate frame. Calculating the apex of the target from this data, we determine the optimal orientation and translation from the fixed three-dimensional frame to each lidar via the least-squares fitting of the two three-dimension apex point sets. Thus we offer a closed form solution without the need for QR decomposition that, from a mathematical perspective, is optimal even in the presence of noise. This method has been proved in both simulation and via a statistical design of experiment. Such a solution may lead to the development of a real time heuristic for determining optimal lidar calibration transformations.

Design, Construct and Test a Computer Controlled Mannequin Mover for Automated Guided Vehicle (AGV) Obstacle avoidance Measurements

David Nahmias

Many warehouses use Automated Guide Vehicle's (AGV) to autonomously move products from shelves to trucks. These commercial robotic vehicles have the potential to be used side by side with humans in flexible manufacturing and with robots onboard. However, before AGVs can begin to be in next generation manufacturing near workers, some questions need to be addressed: How do you test an AGV's ability to maneuver around objects and people? What if the object or person is moving? Should we hope that all of the AGV's systems and obstacle avoidance software are going to work perfectly and have people interact with AGVs without testing? The motivation of this project is to answer some of these questions by creating and implementing a standard test method for measuring the obstacle avoidance performance of an AGV with moving objects similar to a walking person. To do this a Computer Controlled Test Piece/Mannequin Mover (CCTPMM) is designed to be able to control and monitor the position of the Mannequin or Standard Test Piece being moved into the AGV's path. Furthermore, the path of test piece/mannequin motion can be controlled by a computer with the Initial Velocity, Maximum Velocity, Acceleration and Deceleration of the CCTPMM as motion parameters within the LabVIEW program. The CCTPMM is designed so that it is so low to the ground, 1-½'' above the ground, that the sensors mounted on the AGV will sense the Test Piece or the Mannequin before sensing the CCTPMM cart structure. The CCTPMM is controlled by a double spool system attached to a programmable stepper motor and is made to be as lightweight as possible for maximum mobility. To fully simulate motion of a walking person, further research will require a new mannequin with actuated legs to simulate gait which will be mounted onto the CCTPMM. Altogether, this research will form a document to be used as a test method reference for AGVs safety and performance standards.

Detecting Nanoscale Three-Dimensional Shape Variations Using an Optical Microscope

Peter Weck

As the nanotechnology industry progresses, the demand for fast and reliable nanoscale metrology tools grows. The Scanning Electron Microscope (SEM) and Atomic Force Microscope (AFM) are routinely used to satisfy these needs. However, optical methods have the potential to be much faster and more cost effective. Through-focus Scanning Optical Microscopy (TSOM) is a relatively new optics based method utilizing conventional optical microscopes to extract 3-D shape information about targets with nanometer scale sensitivity.

In this presentation, I will discuss how the TSOM method uses images taken by a microscope over a range of focus positions and compiles them to form a 3-D dataset. The experimental results of applying the TSOM method to the analysis of nanometer scale variations across high aspect ratio targets on a silicon wafer will be presented. Analyzing such targets with methods like SEM is time consuming and often requires destructive sample preparation. Furthermore, TSOM is capable of more localized analysis than other optics-based methods like scatterometry, allowing both for analysis of the variation between individual grating targets on the wafer and across a single target. If shown to be reliable and accurate for analyzing nanoscale dimensional variations across such targets, the TSOM method could become an important tool in industrial process control, defect detection, and other aspects of the semiconductor and nanotech industries.

Towson University

Security of WS-Biometric Devices (WS-BD)
Emily Jay

The major goal of the WS-BD project is to improve interoperability of biometrics devices by exposing the biometric sensors to clients over a web service. This method supports interoperability of these devices by eliminating the need for device drivers, and allowing for equal functionality despite differing operating systems, communication protocols, and other common client-specific barriers. While the interoperability is an undeniable benefit, using a web service exposes the personal identifiable information (PII) to a number of potential risks. These risks can be mitigated with the implementation of security protocols that help uphold the confidentiality, integrity, and availability (CIA) of information. This summer, I was tasked with providing input and guidance on security measures and protocols for the WS-BD specification. My research was organized by analyzing three different possible environments for the WS-BD (development environment, isolated network, and public network) at three different layers of the Open Systems Interconnection (OSI) model (network, transport, and application). In this talk, I will discuss the structure of my research, my findings, and the reasons for selecting certain security protocols. I will also briefly describe the process of implementation for each protocol suggested for each environment at each layer, and discuss the possible considerations and hurdles that may have to be overcome for an individual implementation case.

University of California Berkeley

A Review on Additive Manufacturing Processes
Kenneth Hwang

Additive manufacturing (AM) has the potential to create geometrically complex parts that require a high degree of customization using less raw material and producing less waste. Recent studies have shown that AM can be an economically viable option for use by the industry, yet there are some inherent challenges associated with AM for wider acceptance. The lack of standards in AM impedes its use for parts production since industries primarily depend on established standards in processes and material selection to ensure the consistency and quality. An inability to compare additive manufacturing performance against those seen in traditional manufacturing methods is a barrier for implementing AM processes. The scope of this research was to assess the current state of AM and organize the research findings based on different perspectives such as capabilities, materials, applications, process technology, and sustainability.

University of California San Diego

Etch Damage in Magnetic Thin Film Head Materials
Lisa Krayer

The areal density of hard drives have increased at an annual rate of >25% for most of the past 50 years, largely through aggressive scaling of the components - most notably the thin film heads. Continued improvement will require precise sub-nm scale optimization. Of particular interest is the understanding and control of magnetic interfaces created during device processing by etching and milling. It is well known that etching and capping can alter the microstructure, electronic and magnetic properties of the interface, resulting in drastic changes to the net magnetic properties. However, the exact nature of such

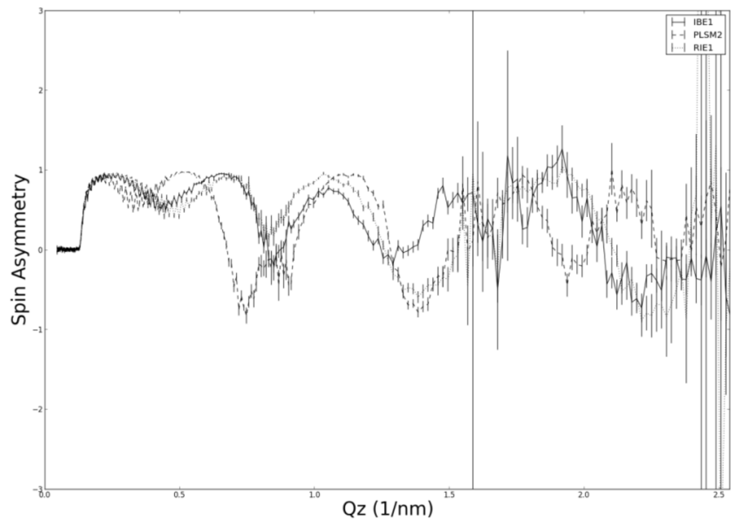


Figure 1: PNR data for CoFeB-based multilayers etched by ion beam etching (IBE), reactive ion etching (RIE), and plasma etching (PLSM).

"dead layers" is not well understood, as the spatial extent of such regions can only be loosely inferred from standard magnetometry techniques. Thus, we have used a spatially sensitive probe - polarized neutron reflectometry (PNR) [1-2] - to measure the nuclear and magnetic depth profiles of multilayers comprised of a common read head material, CoFeB, - etched by different industrially relevant techniques. 5 nominally identical Ta / CoFeB multilayers were sputtered onto Si / SiO_2 substrates, and the top 2 nm of each CoFeB layer was removed using ion beam etching (IBE, low damage), plasma etching (PLSM, intermediate damage), or reactive ion etching (RIE, high damage), before capping with a protective Cr layer. Magnetometry results reveal that etching technique significantly affects the coercive field, ranging from 0.3 mT for RIE to 0.8 mT for PLSM. Using PBR at NIST, spin-dependent reflectivities were measured for these samples in a 5 mT saturating field. The PNR data are shown in Figure 1 plotted as spin asymmetry (the difference in non spin-flip reflectivities divided by the sum), a quantity useful for visualizing the magnetic contribution to the data. Pronounced, etching-dependent oscillations are observed, indicating sensitivity to the samples' magnetic depth profiles. Model-fitting of the data reveal the structural and magnetic depth profiles, allowing us to precisely correlate the thickness, composition, and magnetization of the damaged region with etching technique.

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[1] B. J. Kirby, *et al.*, *Physical Review B*, **81**, 100405, (2010). [2] T. Zhu, *et al.*, *Applied Physics Letters*, **100**, 202406, (2012).

University of Delaware

An Investigation of the Stabilizing Effects of Surfactants on Bio-Therapeutics

Marianna Fleischman

Monoclonal antibodies represent the fastest growing biomolecules in the pharmaceutical field due to their important and life-saving applications. Unfortunately, the high concentrations of proteins required for effective formulations often drives the solutions to aggregate, forming particles and sediment. Particulate formation is often toxic, and can have adverse reactions to the user, including death in some cases.

One of the proposed mechanisms for the formation of aggregates is the exposure of protein therapeutics to various solid-water and air-water interfaces. Surfactant additives have been shown to reduce the occurrence of this undesirable behavior, however, their exact contribution to the phenomena is not well understood. Because both surfactants and proteins are prone to adsorption at interfaces, this competitive binding may reduce opportunities for protein aggregation if it is found that surfactants are favored over proteins for adsorption. Additionally, colloidal stability in the bulk solution may be increased through protein encapsulation in surfactant micelles. X-ray and neutron reflectometry are powerful techniques to study protein adsorption and desorption on multiple surfaces due to their high level of precision in probing monolayers.

Here we present the results of our study on the interactions between non-ionic surfactants and bovine serum albumin (BSA) and immunoglobulin G (IgG1) proteins at multiple interfaces. Using X-ray reflectometry, we are probing the competitive binding of protein and surfactant molecules to the air-water interface and provide a detailed description of the layer formed as a result of these interactions. The effect of multiple dilation and compression cycles of this layer on the solution properties of protein is examined using micro flow imaging (MFI). Finally, we investigate the effects of surfactants in the bulk solution of proteins, containing varying surfactant concentrations, using small-angle neutron scattering (SANS).

Our comprehensive approach will span all potential interaction platforms of proteins in solution and interfaces and thus will provide a better understanding on the link between protein surface association and solution aggregation as well as how and why surfactants may facilitate bio-therapeutic stability.

University of District of Columbia

High-Throughput Photovoltaic Efficiency Testing Rig
Jote Jinfessa

Flexible organic solar cells are a promising technology to harvest renewable energy that can be manufactured at high speed and low cost using patterning and coating methods borrowed from the graphic arts. The processing of an organic solar cell can dramatically impact the materials structure that develops at the nanoscale, with significant impacts on the solar cell efficiency. To understand the effect of material structure on device performance a large set of processing parameters must be explored, requiring a high-throughput testing facility. We have developed a multiplex testing system that will evaluate the solar power conversion efficiency of a large batch of organic solar cells in an automated fashion. This involved designing and constructing the physical setup to make electrical contact with up to 24 devices simultaneously. Additionally, we have written the control software for automated testing of all devices. The final task will be to fabricate and test organic solar cells using our new testing system.

University of Evansville

Performance Testing for Android Devices for Tactical Military Use
Ian Bashor

The Transformative Apps (TransApps) team is tasked with testing tactical software being developed to assist military personnel on operational missions. A subtask assigned to NIST through the sponsor agency Defense Advanced Research Projects Agency (DARPA) is to assess the hardware features of various phones to support the selection of the next handheld used for these purposes. Global

Positioning System (GPS) is one such hardware capability critical to success within tactical environments. The design implementation, and data analysis of GPS testing is a critical element to this selection process. This talk will introduce concepts of how to measure accuracy and Time to first Fix (TTFF) on a GPS unit as well as the process of testing handheld device software.

GPS doesn't work 100% perfect all the time where the two main sources of error are 1) Accuracy 2) TTFF. All techniques talked about use open air/open sky techniques eliminating the need for costly and bulky laboratory equipment. The only required for our testing plan is a few key apps and a ground truth.

Software testing is a repetitive process; our team must test software in every way possible and repeat our processes every two weeks when we get a new build. Because our products are being received by the military all testing must be done with a tactical mind-set, considering both missions and efficiency. Our testing involves working side-by-side with the software developers and military personnel.

The testing done here at NIST by the TransApps team is having a direct effect in the world today. This technology is being implemented in Afghanistan. Currently, over 4000 devices have been deployed since 2011. Likewise, there have been instances where first responders and emergency personnel have leveraged this technology in domestic settings. The ultimate goal is to increase operational efficiency and enhance safety in both combat and non-combat tactical environments.

University of Illinois

Half-Quantized Vortex Molecules in Quasi-Two-Dimensional Rotating Binary Superferrofluids

Wilbur Shirley

Since their realization in 1995, Bose-Einstein Condensates (BECs) have garnered much interest due to their utility in studying macroscopic quantum phenomena. One such phenomenon exhibited by these systems is that of superfluidity, which allows for the formation of quantum vortices in condensates rotating above a critical angular velocity. A large body of research exists on the structure of individual vortices as well as the multivortex configurations found in trapped rotating condensates. In recent years BECs composed of dipolar atoms have been realized, sparking interest in this new direction of research. Dipole-dipole interactions enrich the physics of condensates because of their long-range and anisotropic nature.

Our focus is on the ground state configurations of rotating condensates in oblate harmonic traps composed of two distinct interacting chemical components, in which atoms of one species have a permanent dipole moment. These systems are modelled via numerical simulation of a modified Gross-Pitaevskii equation, in which the ground state is found via imaginary time evolution. For the sake of computational feasibility it is assumed that the condensate wavefunction follows a Gaussian distribution in the polar direction, thus limiting computations to two dimensions while keeping intact distinctly three-dimensional dipolar physics. We have found that under regimes of sufficiently strong interparticle interactions, the addition of dipolar interactions in one species creates a phase in which pairs of half-quantized vortices (a vortex in one component filled by a density peak in the other) in opposite components are energetically bound to each other. These bound states lie in contrast to lattices favored in non-dipolar condensates which maximize the distance between coreless vortices. This phenomenon is explained by numerically modeling the interaction potential between half-quantized vortices in opposite components.

Measuring the Defect Density of Carbon Nanotubes
Philip Trettenero

Carbon nanotubes (CNTs) exhibit extraordinary physical, thermal and electrical properties that can be used for various applications, such as strengthening current materials as well as becoming the backbone for future integrated circuits. CNTs are made from a single layer of graphene rolled into a tube. The angle that the tube is rolled at is called the chiral angle. They can be either metallic or semi conducting depending on the diameter and chiral angle of the tube. Furthermore, CNTs can have one layer or be composed of many walls of graphene rolls. The tubes are respectively called single wall CNTs and multi wall CNTs. Currently, synthesizing specific tubes is quite challenging; defects are also very common in carbon nanotube samples. These defects include changes in tube diameter, bent tubes and unwanted growth on tubes.

This project proceeded in four stages. First, samples were prepared to yield a sufficient number of desired nanotubes. Second, samples were examined using transmission electron microscopy. After collecting the data analysis began, using high level software to define the nanotubes unique characteristics. After the exact type of nanotube had been identified, defect analysis began. Defect analysis combined data from a theoretical model along with a temperature factor in order to match the experimental data. The main goal of this project was to determine a standard method for estimating the error in CNT-composites. Additional goals included improving current software for accurate measurement of defect densities.

Behavior of Fire Fighter Polycarbonate Personal Protective Equipment in Extreme Heat Conditions
Joseph Willi

More than 30,000 fire fighters were injured on the fireground in 2011. Obviously, firefighting is a dangerous occupation, but the level of hazard can be minimized through the improvement of personal protective equipment (PPE) and tactics used by firefighters on the fireground.

In the summer of 2012, a team of researchers from NIST’s Engineering Laboratory Fire Research Division collaborated with Underwriter’s Laboratory (UL) and the Fire Department, City of New York (FDNY) to examine and measure the effectiveness of various firefighting techniques. Over 20 live-fire experiments were executed in 18 townhouses on Governor’s Island in New York. These experiments provided researchers with an extraordinary amount of data concerning how certain fire ground operations affect conditions inside a structure.

The purpose of this project is to obtain and analyze data regarding the failure of specific firefighter PPE, constructed from polycarbonate, due to extreme heat conditions. The data from the townhouse experiments characterized the thermal environment throughout the townhouses. This provides guidance on what conditions should be used for the laboratory scale equipment testing. The laboratory experiments used a high temperature oven to examine the impact of convective heat transfer on the polycarbonate and exposure to a gas fired panel to examine the impact of radiant heat transfer. Comparison and examination of data from these experiments can potentially lead to the creation of better standards for firefighter PPE. Also, the data from these laboratory experiments can be compared to the data from the Governor’s Island experiments to evaluate certain firefighting tactics and demonstrate which tactics would have the higher potential for injury due to high thermal exposures which could lead to equipment failure.

University of Kentucky

Improving the 3-D Metrological Capabilities of the SEM
Benjamin Hackett

The future production of emerging nanotechnologies requires accurate and repeatable measurement of ever smaller 3-D nanoscale features placing challenging demands for the improvement of current instrumentation as well as measurement methodology. The scanning electron microscope (SEM), a common metrological tool used in integrated circuit production, contains shortcomings inherent in its mode of operation that limit the dimensional characterization of nanoscale features. In order to minimize one such source of measurement error, detriment to image resolution caused by instrument stage drift and vibration, the limits and capabilities of drift compensation and image composition techniques were tested to determine optimal instrument parameters for image acquisition. The analysis of the multitude of sources of measurement error and the implementation of a suite of corrective solutions yielded improved image resolution and measurement accuracy.

University of Maryland Baltimore County

Understanding Intracellular Biomineralization: Exploring the Role of pH and Supersaturation of the Composition of Amorphous Calcium Phosphate
Natalie Austin

Bone and teeth are composed of an intimate associate of the mineral apatite and the structural protein collagen. Studies have suggested that amorphous calcium phosphate (ACP) is a requisite precursor phase of apatite during bone formation. ACP formation has been described as the clustering of several molecules of calcium ions (Ca^{2+}) and phosphate ions ($PO4^{3-}$), with an ideal composition of $Ca_9(PO4)_6$ and a Ca/P ratio of 1.5. However, our experimental evidence has shown that ratios deviating from 1.5 are possible. We are interested in understanding how these varied compositions of ACP are formed as well as the consequences of changes in composition on the structure and reactivity of ACP. These results can be used for studies of the bone formation process, biomimetic synthesis of substitutes for bone materials, and dental remineralization applications. To tune the composition of ACP we tested the effect of Ca/P ratio of the precipitating solution and pH on the resulting composition of ACP. In addition the type of wash solutions used to remove excess ions (Na+ and H+ in the form of HPO_4^{2-}) from synthetically derived ACP can also have an effect on the composition of ACP. Our compositional analysis indicates that pH and the type of wash strongly control the ACP composition, but not the solution Ca/P ratio. Whereas our preliminary Pair Distribution Function analysis from synchrotron X-Ray total scattering experiments show that ACP local structure changes depending on ACP deviation from an ideal Ca/P ratio of 1.5 and especially at a low Ca/P ratio of 1.0.

Heterogeneous Mapping Platform for Model-Based System Engineering
Michael Bishoff

Model-based systems engineering (MBSE) is becoming increasingly necessary in the manufacturing world. MBSE benefits from the power of new information technologies to integrate relevant product data into digital product models. Manufacturers need product models that can be shared, exchanged, enriched, and used by many different actors and (IT) systems. There is a large diversity of systems which makes product data integration difficult and often requires mappings between different sources of data. Mapping frameworks already exist but mainly deal with files; whereas many new standards implementations are based on service oriented architecture (SOA) principles because users can easily access a company's service over the Internet.

In my talk, I will describe the software I developed that models and maps any web service data into an Eclipse Modeling Framework (EMF) model. I accomplished this by first generating Java classes that model the web service. Then my software generates a client for the web service. Once the user specifies which services they would like to access, the software calls the web service functions and constructs appropriate XML and EMF files that contain the response data from the web service. The combination of the response data, in an XML format, and the EMF model can then be used in the Eclipse Modeling Framework to allow additional analysis and manipulation of the data.

Monitoring Magnetic Levitation through Interferometry
Vignesh Dhanasekaran

Scientists are currently working to redefine the kilogram in terms of an invariant constant of nature, the Planck constant. However, the experiments in support of redefinition are performed in an evacuated environment. In order to disseminate the new kilogram to the world, there has to be a method to transition from a mass standard in a vacuum to a mass standard in an atmospheric environment.

Direct comparison of vacuum and air masses using a single mass comparator can be accomplished using a magnetic suspension technique to bridge the vacuum-air interface. The mass comparator has a resolution of 10 micrograms, so even small movements affect the stability of the measurement. Since variation in the vertical direction of the suspended mass causes uncertainty in the measurement, the suspended mass must remain as close to stationary as possible. In order to quantify the vertical stability, an interferometry system will be designed to attach directly to the suspension system. The system will be able to detect motion with a resolution of 0.15nm and will also calculate the velocity of the vertical motion. The data read by the system will then be analyzed using a LabVIEW program which will record the velocity, position, and the standard deviation of the movement of the levitation.

Mobility Management for Heterogeneous Networks
Celia Drew

Smart phones. Tablets. Apps. A decade ago, these words were not part of most people's vocabulary. In the last ten years, the number of ways in which people communicate and the number of electronic devices used has grown steadily. But with this much higher usage, cell phone networks are having a more difficult time in managing situations when people with mobile devices move around and need to change the base station to which they are connected. One way to solve this problem is to introduce heterogeneous networks (HetNets for short). Heterogeneous networks provide service to users by incorporating cells with varying coverage areas. Large coverage areas that result from big, high-power cell towers are known as macrocells, smaller towers that cover a college campus or industrial park are considered picocells, and home base stations that are typically connected to the Internet via a coax or Ethernet wall jack and provide coverage over a very small area are called femtocells. If too few cell phone towers are serving an area, the probability of an outage increases. On the other hand, having too many cell towers in a given area can result in a ping-ponging effect where the device constantly switches base stations. This results in a very inefficient use of energy and network resources. The wireless industry is working on ways to reduce these bad effects.

This summer, I have been running computer simulations with the MATLAB programming language and using mathematical analysis to look at how mobile device performance is measured. I validated theoretical results from a Monte Carlo simulation, and I helped improve some code by taking the mechanisms that are used to eliminate ping-ponging and handover failures into account. In this talk, I will explain the importance of the MATLAB files I have coded and the simulations I have run and how they will benefit our technologically growing world.

Growth Factor Deliverable Smart Nanofiber Scaffolds for Tissue Engineering Applications

Neha Kumar

Tissue engineering (TE) represents a paradigm shift in healthcare therapies and treatments by repairing, replacing, or regenerating damaged cells and tissues in the human body. Chemical cues such as growth factors (GFs) and cytokines are the key components in TE with the ability to target specific tissue regeneration. Immobilization and loading of GF into a polymer matrix using a common emulsion method, previously explored in design of scaffolds, have shown only limited success due to the loss of GF's bioactivity during fabrication process and storage, as well as generally low encapsulation efficiency, and uncontrolled release profiles. All of these drawbacks lead to unpredictable therapeutic efficacies of these engineering scaffolds. We developed novel nanoencapsulation of protein into a sugar-glass-matrix to form a protein-sugar-glass nanoparticles (SGnP) system to develop a generic platform for protein (e.g., growth factor) encapsulated scaffolds of any polymer and protein system, preventing protein activity loss against processing and storage stresses, while reaching high loads and exhibiting burst-free sustained release of protein in their active form. To prove our hypothesis, in this study four model, clinically relevant GF; bone morphogenetic protein 2 (BMP-2), fibroblast growth factor (FGF), transforming growth factor beta (TGF-β) and vascular endothelial growth factor (VEGF), were encapsulated in SGnPs and used for fabrication of GF encapsulated nanofiber scaffolds by the electrospinning technique. Chloroform solutions of polycaprolactone (PCL) and poly(lactic-*co*-glycolic acid) (PLGA) and two loading concentrations of each GF (1% and 5%), were used to fabricate the nanofibers scaffolds. The release profile of GFs from nanofiber scaffolds was studied for 30 days. Human bone marrow stromal cells (HBMSCs) were used to study the potentiality of these scaffolds for specific functional tissue regeneration.

Effect of Reduced Beam Divergence on NIST Ozone Standard Reference Photometer Measurements

Peter Luu

Ozone is an oxidizing agent that damages many materials, respiratory systems, and plant tissue. As a pollutant at ground level, ambient ozone levels are monitored at air monitoring stations by commercially produced instruments. These commercial instruments are calibrated by an international network of NIST SRPs (Standard Reference Photometers) acting as primary ozone standards.

NIST SRPs measure ozone concentrations by the absorption of a collimated UV (ultraviolet) beam directed through glass cells containing gas samples. The collimated UV beam in a NIST SRP is known to diverge beyond the inner diameter of the glass cells and to be carried by total internal reflection to the detector. Various optical configurations, using different apertures sizes, gas cell diameters, and source blocks are being tested to reduce divergence. The effect, if any, of the reduced divergence on ozone measurements will be observed to reduce uncertainty in ozone measurements and suggest changes to the SRP.

Creating Profiling Tools to Analyze and Optimize FiPy
Danya Murali

Many physical processes that occur in materials science are governed by partial differential equations (PDEs) including microstructure evolution, electrodeposition and phase boundary motion as well as many more. Solving the governing equations with appropriate numerical methods is a vital part of understanding these processes. FiPy provides a high level interface for posing and solving PDEs (typical to material science) with appropriate numerical methods. It is an open-source, Python based code that both uses and integrates well with the existing scientific Python code stack. Although FiPy is a well established tool, it still requires improvements in both runtime and memory performance as the emphasis during development has tended to focus on usage and functionality rather than efficiency. In particular, FiPy's memory usage limits its capability to handle large simulations. This presentation describes efforts to measure FiPy's performance and identify bottlenecks and then subsequently improve FiPy by optimizing these bottlenecks. An important part of this effort is creating general tools for time and memory profiling that integrate well with FiPy. In particular, the developed tools gather, compile and cache profiling data for many simulations and also produce graphs that show performance scaling against simulation size. Results from these tools are used to locate and improve functions and methods that seem particularly wasteful with memory.

Optimization and Modeling of MIS Devices for Solar Energy Conversion
Nathan Smith

Improvements in the performance of solar energy conversion technologies are necessary to encourage significant and healthy change in the world's energy infrastructure. Photovoltaic (PV) and photoelectrochemical (PEC) solar cells are two solar technologies that could contribute to this transformation, where the former uses sunlight to produce electricity and the latter uses sunlight to produce hydrogen, a storable solar fuel that can later be used in fuel cells. This research focuses on using Metal-Insulator-Semiconductor (MIS) configurations for PV and PEC solar cells in which metallic collectors are positioned on top of an oxide-covered p-type bulk of Si. In order to maximize the energy harvested from the sun with MIS solar cells, many aspects of semiconductor physics must be better understood, and modeling efforts are very important for this purpose. Various design parameters are considered in this work, including the geometry of metallic collectors, the thickness of the tunneling oxide layer, and the addition of surface nanostructures. By initially using MATLAB as an approximation and then using the Python-based FiPy engine for improved accuracy, the influence of changing these various cell design parameters can be analyzed and compared to experimental results. In experimental studies, MIS solar cells are based on a Silicon semiconductor layer due to its low cost, large elemental abundance, and ability to efficiently harvest solar energy. A thin SiO_2 layer serves as the tunneling oxide and the collectors are made by depositing platinum on the surface via electrodeposition (for smaller sizes) or a shadow mask technique (for larger sizes). Through comparison of modeled and experimental performance, a better understanding of device operation is obtained, allowing for the development of more advanced and efficient PV and PEC cells. Key insights obtained from these studies will be reported and remaining challenges in the modeling, design, and development of MIS solar cells will be discussed.

University of Maryland College Park

Resource Public Key Infrastructure (RPKI) Deployment Strategies and Its Impact on Today's Backbone Routing
Guru Ram Ambalavanar

In a world where global connectivity is essential to even the simplest aspects of everyday life, the Internet controls us. Its continued operation is paramount in maintaining the massive machine that is the human ecosystem. From the smallest viral images to the most important bank transactions, we rely on the Internet.

Attacks against the Internet have happened many times already, where traffic of YouTube was redirected to Pakistan, Internet traffic from the United States to Europe was redirected through China, and complete countries such as Egypt were taken of the net.

To strengthen the robustness of the Internet and prevent such malicious attacks, the Internet Engineering Taskforce (IETF) started developing a mechanism to verify Internet route announcements using Resource Public Key Infrastructure (RPKI). This project focuses on the use of the newly developed standard for RPKI route origin validation, which focuses on preventing Internet routers to announce IP addresses that do not belong to them and therefore from stealing / redirecting Internet traffic. For this, NIST has developed a reference implementation called Security Routing Extension (SRx) and embedded this code into open source routers to be able to combat these attacks. The placement of these servers is key, and this project's objective is to find the optimum deployment strategies to determine the maximum impact of protecting against attacks on the Internet. To allow performing impact studies, we use Emulab to generate Internet topologies in which we inject attacks and counter them with strategic placement of SRx servers. The results of this experiment will contribute to the research being done at NIST and the IETF at large.

Computer Assisted Translator for SPAF
Wasson An

Increasing the availability, usability, and effectiveness of modeling and optimization technologies has been identified as a key enabler for improving sustainable manufacturing. However, using such technologies, especially for small and medium sized enterprises, has faced a major challenge. Complex sustainability analysis requires formalization by simulation tools and/or an optimization modeling, which needs significant expertise and substantial implementation. To satisfy the industrial needs, NIST proposes Sustainable Process Description Analytics Formalism (SPAF), which provides a mechanism to represents the knowledge of process flow, data, and mathematical specification for sustainability analysis and optimization. In order to utilize this mathematical and analytical formalism efficiently and automatically, a translator is required to transform the models developed using SPAF to computer-interpretable and understandable format that can be used by commercial simulation or optimization tools.

My project is to create a graphical user interface to assist in creating SPAF. The interface will allow for the easy creation of SPAF. The goal is to allow common industry users to generate SPAF quickly and easily. The graphical user interface (GUI) is designed using standard software engineering principles such as UML diagrams. After designing the interface, I started to create a prototype to implement into a test bed.

Cryptography in Constrained Environments
Andrew Badger

The prominence of small-scale computing in our daily lives has given rise to a new requirement in cryptography. Many small low-power devices have highly limited memory and processing power, but still require security in their data transactions; a few examples are wireless headsets, security badges, and pace makers. As a result, significant research has gone into developing light-weight secure cryptography. This research project evaluates the relative effectiveness of Keccak, SHA2, Simon, Speck, and AES when applied to securing a network of temperature recording microcontrollers.

After implementing MAC authentication with this mix of hash functions and block ciphers, we evaluate their footprint in terms of memory and processing time. From this data, we can estimate the battery life of the specific configuration. This information allows us to select efficient cryptographic algorithms when working with different microcontrollers.

Along with implementing cryptographic algorithms, we developed utility applications using the iPhone SDK; these iPhone applications allow users to compute the various algorithms we used for MAC authentication and monitor our network of microcontrollers. These small applications are useful references for future implementers of these algorithms and allow for a more interactive demonstration of our findings.

This research will help people select algorithms to provide security for microcontrollers, embedded devices, and other small platforms. In mobile computing there is always a balancing-act between security, performance, and cost. Our goal is to help developers find the correct balance when working in constrained environments.

From Web Graphics to 3D Haptics: Depecting Web Images for the Blind and Visually Impaired
Andrea Bajcsy

How would you surf the Web and perceive digital images if you were visually impaired? Currently, many companies around the world have designed specialized auditory navigational systems for blind people using computers. However, there is still a gap in how to deliver the information found within 2D Web graphics to blind individuals. One of the applications that demonstrates this gap is the access to election data and statistics which use graphs and maps to illustrate trends.

In order to address this problem, we have designed a workflow of automated computational steps which translate 2D graph and map images into 3D printed models. In order to validate the accuracy of the computational workflow, we have developed and labeled a reference database containing 676 images downloaded from election and voting-oriented webpages. The workflow consists of several modules: a HTML Parser, Image Type Classifier (Graph vs. Non-Graph), Graph Type Classifier (Bar chart vs. Pie chart vs. Line chart vs. Map), Color-to-Elevation Mapper, and a STereoLithography (STL) File Generator to produce 3D Computer-Aided Design (CAD) models for 3D printing.

Based on the current workflow steps, we were able to (a) extract all image files from downloaded webpages, (b) achieve 92% accuracy for the Image Type Classifier using Color Histogram-based analysis, (c) design a Bar chart identifier, (d) prototype multiple Color-To-Elevation conversion methods, and (e) produce STL files of the desired image information as required by 3D printers. The current prototype has been implemented in Java so it can be streamlined and can run on any operating system.

In the future, we envision multi-sensory representation (auditory combined with tactile sensing) of Web graphics for blind Web users. Furthermore, we would like to expose blind individuals to these capabilities and optimize the tactile and eventually haptic representation of Web images.

Characterization of Microfabricated Particles and Protein Aggregates Using a Custom Microfluidic Coulter Device

Shir Boger

A major challenge during formulation of therapeutic proteins is overcoming their limited stability caused by various factors including pH, shear, and thermal stress. Current research has suggested that the presence of protein aggregates is considered to be undesirable due to potential immunogenic reactions and other adverse effects. There has recently been an increased focus on characterizing these protein particles, as the exact levels of protein aggregates that lead to enhanced immune response is unclear. Other labs have found that current market devices provide different distribution and count for aggregated proteins which has led to a lack of standard measurement of these aggregates. My project involves using a custom microfluidic Coulter device to characterize microfabricated particles of controlled shape particles (beads and rods) as well as protein aggregates. The application of the Coulter principle is a well-established method for counting and sizing particles in which objects are placed in an electric field and modify the current flow in that field. As particles pass through a constriction, electrical pulses are generated whose magnitude is proportional to the particles' volume. Additionally, the electric signal photographs an ultrafast light flash which is used to photograph the particle. A background image of the channel is then used to isolate the particle and compute parameters regarding its size distribution. The results obtained with the microdevice will be compared among the control shape and protein aggregates and with those from conventional equipment.

Thinking Green: Sustainable Energy Modeling for Arc Welding Processes

Kevin Chuang

Much emphasis exists for the conservation of energy usage among a product's life cycle. However, a bulk of energy consumption takes place in the manufacturing sector, prompting efforts to standardize the energy flow through a plethora of manufacturing processes. Many attempts have been made to tackle this overarching issue with none accomplishing full generality thus far.

The Engineering Laboratory at NIST is developing an energy calculator designed to allow clients to model energy flow in assembly processes and eventually entire production plants. My colleagues and I focused on modeling the 6 most dominant arc welding processes: flux cored, gas metal, gas tungsten, shielded metal, submerged, and plasma arc welding. We developed a graphical user interface (GUI)-driven energy calculator that models energy flow and loss through welding systems consisting of not only the welding equipment but also critical auxiliary processes.

In this talk I will differentiate between the arc welding processes as well as divulge into a variety of joints and grooves that the welding acts on. An in-depth energy analysis of the processes along with the associated enabling equipment will follow. Lastly, I will tie the loose ends and relate our efforts with the general goal of the project.

Creating an Efficient Program to Simulate Dynamics of One-Dimensional Quantum Many-Body Systems

Justin Clagg

With the great progress in quantum information and quantum control of quantum many-body systems, such as the ultra-cold atom systems, creating efficient ways to simulate the dynamics of quantum many-body systems has become increasingly important. My project is based on a recently introduced method, the time-evolution block decimation (TEBD) method. This method has shown to be an efficient way to simulate one-dimensional quantum many-body systems. The main goal of my project is to create a programming code for the TEBD method in C++ based on an existing code in Fortran. The created code is bench-marked against the existing code to ensure accuracy and computational efficiency. We also apply the code to simulate the dynamics of a one-dimension lattice system of ultra cold atoms.

Durability of PET in Photovoltaic Applications

Kathryn Connolly

The paucity of standards for quantitatively characterizing the performance and predicting the service life of polymeric materials and components used in photovoltaic (PV) systems hinders the innovation, development, and application of PV technologies. The success of PV technologies will ultimately depend on a clear demonstration of their long-term reliability. Currently the scientific basis to assure the PV products meet the 25-30 years of life-time warranty is scarce. In addition, current standardized test methods used for quantifying long-term reliability of PV polymers do not apply the relevant environmental stressors simultaneously. Therefore, there is little knowledge of the synergistic/antagonistic relationships between the environmental factors. Polymer materials are widely used as the backsheet of PV modules, which provides mechanical support for the module and protection from environmental conditions, such as UV irradiation, temperature, and humidity. The backsheet is a multilayer polymer, which traditionally consists of layers of fluoropolymer, an adhesive known as ethyl vinyl acetate (EVA), and polyethylene terephthalate (PET). The degradation of these polymeric materials in the backsheet will eventually lead to the failure of the PV module. In this study, the durability of PET, the material which makes up the bulk of the multilayer backsheet materials, is investigated under exposure to the NIST SPHERE (Simulated Photodegradation via High Energy Radiant Exposure) at three temperatures (55 °C, 70 °C and 85 °C) and 60% RH with simultaneous UV irradiation. The chemical and physical degradation of the backsheet polymer over periodic exposure times is analyzed through the use of Fourier Transform Infrared Spectroscopy (FTIR), UV-Vis Spectroscopy, Atomic Force Microscopy (AFM), and Confocal Microscopy. The kinetics of the chemical degradation of the materials and its correlation to the exposure conditions will be analyzed. The data will provide a better understanding of the durability and lifetime of PV backsheet polymers which can then be applied to PV product development.

Indentation Metrology for Nanomechanical Properties

Luis Correa

There is an increasing demand for reliability of indentation used in determining mechanical properties of micrometer-scale and even nanometer-scale specimens. This is a consequence of advances in the research and development of thin films and nanomaterials in the last few decades. Meeting this demand requires precise and reliable indentation measurements at very low forces and depths, which are measured by nanoindenters. Most commercial nanoindenters suffer with frame compliance and thermal drift, which compromise our ability to test time-dependent properties of materials and make repeatability a challenge. Frame compliance is the deformation of the indenter's frame in response to indentation force, while thermal drift refers to relative motion of the indenter tip and specimen resulting from thermal expansion and contraction that is unknown and uncharacterized. Both effects can introduce error into the force and displacement measurements that are used to determine the mechanical properties of the specimen. An effective method for eliminating these undesirable signals is indentation by surface tracking, where the indentation depth is calculated using the specimen's surface as reference.

This summer I worked on the Precision Nanoindentation Platform (PNP). This is a one of a kind instrument that aims to build metrological standards for nanomechanics. The PNP uses quartz crystal oscillators to track the specimen's surface during indentation, eliminating frame compliance and reducing thermal drift issues. Last year, we demonstrated that the PNP is capable of producing repeatable indentation data, and proved that surface-referenced indentation depth measurements can account for movements of the specimen perpendicular to the plane of indentation. This year our goal is to demonstrate the PNP's ability to measure time dependent properties (creep) using poly (methyl methacrylate) and polyurethane, which are materials known for their viscoelastic properties. A description of how the PNP works and the results from the summer research will be presented at the colloquium.

Database Automation by Solving Puzzles!!!

Syed Elahi

Every year NIST organizes an event called "Take Our Daughters and Sons to Work Day." On this day, children between the ages of 9 and 14 not only witness what their parents do at work, but more importantly they also get an opportunity to be thrilled by the sheer innovations of their parents. Although this event started in 1994 with only 40 children, by 2013 this event had attracted about 300 children. Quite naturally, the level of complexity in organizing this event has immensely increased over the years.

My project this summer has been to tackle these complexities and automate a database that contains kids and their sponsors' information along with information on guide volunteers and presentations. The constraints that I need to work within is that every student group must have a 50/50 gender split, children are placed in a group based on his or her age, the volunteers' availabilities, and ensuring a child does not see same presentation twice even if they have been in the program for five or six years. These constraints make this automation process a big puzzle. Some of the steps that I have taken to solve this puzzle are: 1) drawing an algorithm flow-chart 2) getting introduced to Visual Basic programming language 3) coming up with a set of code to automate the database fields.

In the end, the final set of computer code that my project is intended to produce will have three major advantages. First, it can be run in years to come. Second, it will substantially reduce the manual labor that goes into scheduling. Third, it will generate the event schedule with virtually a couple of clicks of a mouse button.

The Importance of User-Friendly Interfaces for Public Resources
Rena Elkin

The Engineered Fire Safety Group's research is intended to improve safety awareness, prevention, and emergency protocols. If utilized correctly, the division's Web page allows researchers to publicize their findings concerning egress-related topics as well as evacuation-modeling software that they have developed. In order to efficiently disseminate the information, it is crucial to consider the human-computer relationship. CommonSpot is a Content Management System that NIST uses to track and manage corporate Web sites. This computer application provides a uniform appearance among various pages and is organized with a taxonomy of topics that allows for easy navigation by users. Using this application, the Web page was designed to display the optimal user-friendly interface. In addition to increasing data and report accessibility, the Web site also provides an online interaction with outside groups working in the field of egress via Google Discussion Groups. This feature allows the Engineered Fire Safety Group personnel to better distribute their information and answer any questions that the public may have.

In this presentation I will discuss the relationship between human behavior and ergonomics that affect websites' or programs' usability. With this insight in mind, we will briefly analyze the Web page and I will elaborate on how adding various elements were conducive to creating the user-friendly configuration. As can be expected of all computer applications, CommonSpot has its limitations that I will comment on.

The concepts behind designing the Web page also apply to the software that it advocates. As can be found on the Web page, the Egress Estimator is a simulation tool that calculates how long a population will take to evacuate a building. This presentation will conclude with an assessment of the Estimator's current interface and suggested modifications to improve usability. This software exemplifies an important goal in EL/Fire Research - circulating results and designs to engineers and scientists who can benefit from publications, data, and simulation tools to design safer buildings. Technology is only as efficient as the user is proficient in using the device. Therefore, to promote the Engineered Fire Safety Group's research, the Web page and software is designed specifically to cater to its users' needs.

Improving Sustainability Analysis of Unit Manufacturing Processes
Ryan Etkins

Manufacturing accounts for approximately 20% of energy consumption in the United States. As energy consumption and other environmental issues become increasingly high profile, it is important that industry has methods of designing and improving manufacturing processes with an eye for these problems. Current Life Cycle Analysis (LCA) tools and Life Cycle Inventory (LCI) databases can do sustainability analysis based on industry averages. This does not help manufacturers analyze sustainability at the shop floor level for effective decision support, as machine/tool parameters may vary greatly from user to user. NIST has been developing unit manufacturing process models to calculate process energy efficiency on the fly to be used for manufacturing process simulation.

The purpose of this project is to develop a conceptual information model for unit manufacturing processes and create a software prototype that will help to verify the unit manufacturing process models developed by NIST. The software includes a graphical user interface (GUI) that industry could utilize to collect machine and tool performance data and provide their mapping relations to unit manufacturing processes. This enables more accurate design and analysis of sustainable manufacturing processes.

Multi-Substrate Flammability Reduction Using a Layer-by-Layer Assembly with Natural Materials

Nicholas Faenza

Every year fires are the cause of numerous injuries, deaths, and massive amounts of property damage. In 2011, almost 1.4 million fires were reported in the United States. These fires caused over 3,000 deaths, more than 17,500 injuries, and almost $12 billion in property damage. Polyurethane foam is a major factor in the potency of many fires because of its common use in consumer products and its highly flammable nature. Polyurethane foam used in mattresses is the cause for thousands of fires and hundreds of deaths each year. To reduce the number and potency of these fires the flammability of polyurethane foam needs to be significantly reduced. Furthermore, it is important to address health and sustainability issues by using natural materials.

Two common methods for reducing the flammability of foam are to utilize a barrier fabric and to make the foam inherently flame retardant. A layer-by-layer (LbL) assembly method allows the deposition of nanometer thick coatings on foam and fabric substrates. All of the samples fabricated consisted of natural materials such as; Chitosan, Sodium Alginate, and Montmorillonite, which make the coating sustainable and environmentally friendly. The samples were mainly characterized by open flame tests, and a cone calorimeter, which measures the heat release of a burning sample over time. When burned, the coating can form a protective char around the foam, or release non-flammable gases which prevent oxygen from reaching the sample. The coated samples showed significantly improved flammability characteristics when compared to the untreated foam.

This presentation will cover the extent of polyurethane foam related fire damage, the layer-by-layer assembly process, and the coatings used to reduce the flammability of the foam and fabric. The testing methods utilized and the results obtained will also be discussed.

Content-Based Image Comparison

Cynthia Gan

How similar are two images? The answer to this seemingly trivial question actually varies with context, human expertise, and perception. The challenges in automating this process lie in aligning qualities perceived by humans with quantitative measurements. A quantitative method of comparing images would require (1) a system of representation capable of handling diverse types of images with different resolutions and value precisions, (2) a set of image descriptors and (3) a set of comparison measures. Aligning quantitative measurements with human experts' judgments would allow the process to be automated and could save hours of tedious work.

In this project, we addressed the first task, image representation, by implementing several image transformations and extending the NIST internal image comparison service, Versus. The image transformations include the Fourier Transform (FT), red-green-blue (RGB) to hue-saturation-value (HSV) color space transform, principal component analysis (PCA), and Hough transform. We addressed the second task by applying existing histogram and pixel-based image descriptors to said transformations, and the third task by re-using about 60 previously implemented comparison measures. To align these measures to expert valuations, we first generated a set of synthetic images that represent controlled modifications of image content such as position, shape, and texture. We then processed this set with the developed comparison system. The resulting image comparison values can be related to specific content changes and thus with user-specified similarity qualities. In the future, we plan to apply the developed image comparison measurements to images of surface materials and live stem cell colonies.

Electrical Modeling of the Change in Resistance in Through-Silicon Via Daisy Chain Subjected to Thermal Cycling

Fardad Golshany

Three-dimensional integrated circuits (3D-IC) are modern electronic chips in which multiple layers of active electronic components are integrated and stacked vertically into a single package. In advanced 3D packages, through-silicon vias (TSVs) are used to achieve vertical connections between the different stacked chips. TSVs enable high performance devices due to the high density of the vias and the shorter path length of the connections. TSVs also carry relatively higher current densities. However, the reliability of these interconnects are not fully characterized nor understood. A significant issue regarding the reliability of TSVs is the degradation of copper-filled vias through the formation and growth of defects due to thermal fluctuations of the IC, resulting in the deterioration of the propagated electrical signals. Performed experiments have shown that the low frequency (DC) resistance of TSV daisy chain scaled with increasing number of thermal cycles. Physical analyses of thermally cycled TSV daisy chains revealed the occurrence of different defects at different failure sites. However, the contribution of each defect type and its location on the measured resistance change with thermal cycling is not understood.

To understand the contribution of each isolated defect type and its location to the change of DC resistance in TSV, electrical numerical analysis was performed on the COMSOL Multiphysics platform. In this study the different defect types and their locations were defined and modeled. Afterwards, their contributions to the change in resistance were determined and correlated with the performed experimental study. Voids in the TSV were found to have the least impact in the change in resistance with thermal cycling, as void size scaled linearly with resistance. On the other hand, cracks at the TSV-metallization interface, which lead to a change in the contact area, were found to have the most impact on the change in resistance, as the TSV daisy chain resistance was observed to increase exponentially with a decrease in contact area. This observed non-linearity is attributed to the occurrence of current crowding.

Optimizing 3D Structures for the NIST Chemistry WebBook

Kathryn Hafner

Our mission this summer is to enhance the National Institute of Standards Technology's (NIST) Chemistry WebBook (WB) by performing quality control on its contents and by adding 3-Dimensional (3D) structures. Eight thousand people use the WB on a daily basis; it is a highly-trusted free resource for scientists and students around the world and contains data from many collections, beginning with a boiling point measured in 1813. Currently approximately 114,000 chemical species represented in the WB, but only 27,000 have a verified 3D molecular structure. Our goal this summer is to optimize 15,000 structures and add them to the WB. In addition, we are optimizing 6,000 biochemical molecules from the DrugBank, a pharmaceutical and chemical database, and integrating their chemical information into the WB. Our work is relevant because it diversifies the WB, ensuring its sustainability and credibility for the years to come.

The 3D optimized structures were optimized using Gaussian, a quantum chemistry computer code. Our calculations consist of a series of optimizations, progressing from a simple to a rigorous, time-consuming method. In the first method, a classical (balls and springs) molecular mechanics method (MM2) is applied to give a reasonable starting molecular geometry. The second method is the "semi-empirical" method (PM6), which, unlike MM2, considers electron interactions. Optimizations performed using this method take minutes to optimize and yield a good starting structure from which more complex calculations can be made. The third and most rigorous optimization applies density functional theory (B3LYP) and gives a more accurate and robust optimization. In addition to Cartesian coordinates, the computation returns other useful information such as vibrational frequencies which can be compared to experimental measurements or used as a basis for calculating thermodynamics quantities.

Our other task has been to verify the chemical information that is currently in the WB. Each chemical species has basic identifying information such as one or more names, Chemical Abstract Service (CAS) number, molecular weight, chemical formula, and 2-Dimensional structure. We confirm that the WB information is correct, and when necessary, suggest changes or corrections. Our work this summer ensures the WB's sustainability and quality, as well as diversifies the overall database.

Estimating the Cost of Inadequate Interoperability for Manufacturing Processes

Adrian Hamins-Puertolas

Inadequate interoperability is the failure of systems and users to seamlessly exchange information. This inefficiency causes an economic loss of billions of dollars each year for manufacturers and consumers worldwide. In turn, this leads to increased costs associated with design and production, as well as delayed release of products. Many manufactures are harmed by a lack of seamless information exchange in the design and fabrication stages of production, and may be unaware of the high costs of inadequate interoperability, which are often built into the total cost of products by manufacturers. Providing organizational units with an estimate of their cost burden of inadequate interoperability allows the organization to responsibly react to the interoperability problem. This talk will focus on a tool created to provide users with the ability to measure the cost of inefficiency caused by interoperability problems on their manufacturing organization, as well as metrics created to measure the costs of inadequate interoperability.

COMSOL Simulation of Multi-Level Interconnects for Advanced Integrated Circuit Design

Emily Hitz

As demands in the semiconductor industry call for further miniaturization and performance enhancement of electronic systems, the traditional planar (2D) electronic interconnection and packaging technologies show their difficulties in meeting the ever-advancing standards of the industry. To overcome such limitations, 3D Stacked Integrated Circuits (3D-SICs) draw tremendous research interests and have been widely studied. However, 3D-SICs still face some challenges, such as Through Silicon Vias (TSVs) and Back-end of line (BEOL) issues. Consequently, a better understanding of the electric and magnetic fields as well as the capacitances between multi-levels of metal lines can assist in the future design of 3D circuits regarding cross-talk and reliability issues.

From the metrology point of view, the traditional Scanning Probe Microscopy (SPM) technologies show mature capabilities of acquiring the surface metrology. However, additional features such as subsurface imaging are crucial to support the development of 3D-SICs. Recently, several techniques, such as Scanning Microwave Microscopy (SMM), Electrostatic Force Microscopy (EFM), and Kelvin Probe Force Microscopy (KFM) have shown promising capability of subsurface characterization on various semiconductor devices, which would enable observation of current carrying lines beneath a passivation surface.

To enhance our SPM subsurface metrology capabilities and determine more accurately the limitations of the technique, we will compare experimental and simulation results. A multi-level test chip with several well-known buried structures has been designed and will be integrated on a thumb-nail size chip. Pads will be bonded on a printed circuit board (PCB), allowing external bias accesses. Different feature components can be biased separately to simulate a Device Under Test (DUT).

Extensive preliminary investigation of the chip design will be accomplished through COMSOL E&M software simulations of the time-varying electric and magnetic fields of test structures to predict their behavior prior to fabrication. After a test design has been finalized and the test chip fabricated, we will begin characterization of the existing device structures using SPM techniques.

Microelectromechanical Triaxial Accelerometer Testing
Eric Huang

Micro-Electro-Mechanical Systems, or MEMS, is a technology for manufacturing highly miniaturized mechanical and electro-mechanical devices using methods that are similar to those used to manufacture computer chips. The expanding universe of new applications for MEMS inertial sensors includes smart phones, tablet computers, and new wearable sensors for measuring workout intensity. The triaxial accelerometer is a key component of MEMS inertial sensors.

To test MEMS triaxial accelerometers, we will parameterize their output signals for comparison with parameter values derived from independent knowledge of stimulus motion. The accelerometers will be moved on pre-determined paths, and the outputs of the accelerometers will be processed and analyzed by comparing the measured and programmed paths.

For this project, a CrustCrawler AX-18A Smart Robotic Arm test bed was assembled and programmed to move an accelerometer along various paths. The robotic arm was programmed using RoboPRO TASKS, and the data from an Analog Devices ADIS16375AMLZ accelerometer was collected using IMU Evaluation and then exported into Excel for further analysis. This analysis uses double integration of the accelerometer data to obtain position data for comparison with paths established by the programmed movement of the accelerometer by the robotic arm.

The outcome of this project will be a new Nanoscale Metrology Group capability to test a wide variety of MEMS triaxial accelerometers using the new robotic arm test bed with software for generation of programmed paths.

Exploring the Sapphire Whispering Gallery Thermometer
Arec Jamgochian

We are developing a novel temperature sensor that utilizes temperature-dependent frequency changes in whispering gallery modes of crystal sapphire resonators to accurately measure temperature, with uncertainties of ≤10mK. The Sapphire Whispering Gallery Thermometer (SWGT), which is resistant to mechanical shock, would render the more fragile standard platinum resistance thermometer (SPRT) obsolete in industrial settings. We explore whispering gallery modes between 10 MHz and 20 GHz for different variants and configurations of the monocrystalline sapphire cylinder, which acts as a uniaxial, dielectric resonator. Some configurations yield modes with Q-factors as large as 1,000. By tracing the modes' movements as a function of temperature, specifically tracing the peaks, one is able to form a temperature portrait over a wide temperature range which shows that mode peak frequency is inversely linear with temperature. Using this method we are able to automate calibration for these sensors.

This talk will go into detail on some of the different sapphire variations and configurations used, as well as the different methods that were utilized to find the modes, and measure and track their movements.

Graphitic Carbon Thin Films for Neutron Reflectometry Investigations of Rechargeable Batteries and Fuel Cells

Benjamin Jones

Our research pursues the fabrication and characterization of smooth graphitic carbon thin films with various crystallographic morphologies and orientations to enable neutron reflectometry, NR, investigations of electrode intercalation and interfacial effects in rechargeable batteries and fuel cells.

Current methods are limited to CVD production of graphene (single or multiple layers) which roughens the underlying surface. Alternatively similar layers of graphene can be lifted off and transferred to a surface, however this process can introduce buckled layers and contaminants. Another approach is to oxidize graphene to exfoliate it and enable it to be dispersed in water, deposit a thin film of this dispersion and then partially reduce it in hydrazine, which introduces considerable defects and requires a toxic, carcinogenic solvent. These films are incompletely reduced, retaining significant amount of oxides, and are also too rough for detailed NR measurements.

We collaborated with Dr. Dorsa Parviz and Prof. Micah Green from the Department of Chemical Engineering at Texas Tech University, who have discovered a way to stabilize graphene in aqueous solutions using sulfonated pyrene. This dispersion method is significant and novel. Sulfonated pyrene is pi-bonded to the graphene sheets as they are exfoliated from graphite. The charge of the sulfonic acid group keep the graphene dispersed in aqueous solutions up to a determined concentration limit. This process does not require oxidation and the sulfonate groups can be easily removed by carbonization at modest temperatures (750C). The most significant difficulties with this method are the difficulties in solution casting uniform smooth films from dilute aqueous dispersions. We developed methods to fabricate thin films of graphite using this dispersion provided by Parviz and Green, and characterize them using x-ray reflectometry and other methods to determine their compatibility with NR investigations of battery and fuel cell electrodes.

Stampeding Over Cement: Simulating Chemical Kinetics in Parallel with HydratiCA

Kevin Keller

Concrete is the most widely used man-made building material in the world. Despite its ubiquity, hydration mechanisms of the cement binder are not well understood. NIST is developing a computational model, HydratiCA, to study cement paste hydration reactions and microstructure development. This model uses kinetic cellular automaton algorithms to simulate the coupled reactions and mass transport stochastically. Throughout the course of the summer, we hope to finish two projects using HydratiCA. The first is an exploration of early-age cement hydration in which we seek to explore how the dissolution of tricalcium silicate and the precipitation of calcium silicate hydrate gel affect the hydration rate of cement. The second is an analysis of how micro-fillers can regulate the hardening of cement. The complexity and number of calculations involved with these simulations makes them very computationally intensive, so we are using Stampede, the sixth fastest super-computer on the top 500 list, to carry out our experiments. From these projects we hope to emerge with a better understanding of early age hydration mechanisms and to develop a tool for helping with the proportioning of micro-fillers and concrete.

Flexible Conducting Polymer Actuators for Cell Stimulus Applications
Mian Khalid

Human vascular cells are constantly exposed to shear stress and mechanical strain caused by blood flow. This cumulative effect has been demonstrated to have an impact on the expression of certain critical growth factors. The mechanical stimulation of cells can be studied by fabricating versatile conducting polymer (CP) actuators. CP actuators are volume-changing elements: upon application of a certain voltage, the ion or solvent flux swells or shrinks the polymer. CP actuators are biocompatible, operable at low voltages (<1V), and easy to fabricate. Electrodeposition was used to deposit the polymer i.e. polypyrrole (Ppy) doped with dodecylbenzensulfonate (DBS) to a gold film. Voltage, time, and counter-electrode materials were varied to record the effect on Ppy film thickness and homogeneity. Film microstructure and thickness were analyzed with scanning electron microscopy (SEM) and profilometry. NIH-3T3 fibroblast cells were grown on the Ppy surface. Fluorescent staining was performed to assure biocompatibility of the NIH-3T3 cells with the deposited Ppy. Future work will involve integrating Ppy, deposited on a flexible substrate (thin polyethylene terephthalate, PET), with NIH-3T3 cells, allowing for mechanical stimulation of the cell culture.

Metrology of Force-Based Control for Robotic Assembly
Byung Kim

A new class of light weight robots is emerging that utilize force sensing capabilities to enable collaborative robotics in that they sense inadvertent contact with humans. My internship was focused on the development of measurement science to support the characterization of industrial robots having force control capabilities that are used to limit forces in collaborative robots and perform assembly operations. My first assignment was to learn ProEngineer and design two new assembly artifacts that integrate onto an existing force based measurement system that incorporate a 6-axis load cell. These include a reconfigurable gear system and a shaft and retaining ring system that support gear alignment and snap fit assembly operations respectively. The remainder of my internship was spent leading an effort which included a summer high school volunteer to test the force characteristics of a KUKA Light Weight Robot (LWR), an advanced 7 degree of freedom robot with intrinsic force sensing capabilities. These efforts included programming the arm using the KUKA Robot Language (KRL) and experimentation using the LWR stiffness variables test characteristics such as force set point, settle stability, obstruction stability, control switch stability and surface cohesion, a set of performance metrics and associated test artifacts being developed at NIST. Force was collected in two different ways: from a 6-axis load cell fixture under the artifacts and from the force system within the KUKA LWR via a serial port interface. In addition, we characterized the KUKA during these certain tasks and assisted the documentation in defining the capabilities of these robots. We also worked toward developing KRL programs to support testing using the assembly artifacts. Test procedures were developed while perfecting the force control and assembly tasks. These results will aid assessment of robot force control performance and safety measures for human-robot interaction.

Raman Analysis of Carbon Nanostructures
Nadav Kravitz

Carbon nanostructures, particularly graphene and carbon nanotubes, are nano-scale atomic structures composed solely of carbon atoms and exhibit remarkable electrical, mechanical and optical properties. They show great promise in science and technology, for use in transistors, integrated circuits, photovoltaics, touch screens, medicine, and textiles, among many others; as well as in metrology as a reference material. As one may expect, NIST is involved in the standardization and characterization of these nanostructures, which will serve as the backbone of many upcoming technologies. A powerful method for probing nanostructures is Raman spectroscopy, in which a sample is irradiated with visible laser light and the inelastically scattered light is then analyzed to determine molecular structure and composition. Typically, hundreds of individual spectra are required for detailed quantitative analysis of even simple nanostructures. Proper analysis also involves removing background signal, smoothing and fitting spectral features with mathematical distributions to determine their underlying physics. Performing these complex mathematical algorithms by hand on each individual spectrum is a rate limiting step in achieving in-depth analysis on critically important samples.

The goal of this project is to develop a multipurpose and adaptable suite of MATLAB analysis tools and apply them to characterizing samples of carbon nanotubes and graphene. The project also strives to implement a co-located, tuning-fork atomic force microscope (AFM), which will be used to add topographical information to the spectroscopic measurements. As an ambitious goal, the project will combine the two techniques in tip-enhanced Raman spectroscopy (TERS), which involves taking AFM and Raman data simultaneously. This would not be a trivial endeavor, and may require efforts extending into the academic year.

Hand-Arm Coordination: Integration and Control of Dexterous Robots
Gregory Krummel

The coordination of motions by the human body is a trivial requirement for daily functions, including tasks as simple as picking up an object. Accurate and repeatable coordination is necessary for rapid manufacturing, assembly, and mobile manipulation when using multiple robotic devices such as robot arms and manipulators. However, this level of coordination is often difficult to achieve and measure since separate manufacturers use proprietary hardware and software, and the individual systems are usually controlled separately despite being physically integrated.

This talk will summarize the development of a coordinated control interface for a KUKA LWR4+ robot arm and the Schunk Dexterous Hand manipulator. These devices are controlled through separate programming languages on separate hardware, so the interface was designed to operate as a middle-man on a separate server to send movement commands and data requests in parallel and coordinate the two devices to operate in unison or precisely asynchronously. Since the devices operate at separate communication and movement speeds, the calibration of this interface required robot dynamics profiling to identify how each system operated and algorithms to convert these profiles into operation alignment controls.

This coordinated control interface is used for the development, assessment, and validation of performance metrics for coordinated heterogeneous robotic systems. These metrics are based off of existing industry standards on system usability, reliability, and interoperability. In addition, metrics required for coordinated control that are not previously standardized are developed and assessed based on the arm-hand coordination methods in this project. These methods and metrics for coordinated control can be generalized and applied to coordinate and control a wide variety of integrated robotic systems in industry.

The Effect of the Hydration Layer on the Small Angle Scattering Data of Proteins

Anita Kundu

Molecular dynamics (MD) simulations are a powerful tool for modeling proteins and other biomolecules and their interactions with the solvent. Small-angle scattering profiles can be calculated from atomic positions obtained from MD trajectories. To adequately predict scattering profiles one needs to take into account the scattering from excluded water; which is the water displaced by the protein. In addition, water surrounding the protein interacts with the molecular surface is known as the hydration layer. This water has been found experimentally to have different properties than those of the bulk water and must be taken into account when calculating certain small-angle scattering data. Our first goal is to evaluate MD simulations with explicit water to understand the sampling and relative scattering of protein, excluded water, and hydration water. This information will eventually be used to develop methods to account for solvent scattering corrections in order to quantitatively calculate scattering from protein structures.

We have found that the predicted scattering of excluded water and hydration water depends on the orientation of the protein in a water box and the fluctuations of the protein atoms in its trajectory. This project aims to find the best way to include water in these scattering calculations to account for changes in the hydration layer. In order to do this, we chose eighteen different proteins with a variety of chemical properties to study. Using molecular dynamics simulations and a program called SASSIE, we calculated the small angle neutron and x-ray scattering of each protein and its hydration layer as well as the scattering of the excluded water in order to obtain a precise representation of contrast. With these results, we are determining the proper way to incorporate water into the calculations of small angle scattering data, taking into consideration proper sampling of fluctuations of solute and solvent atoms and their effects on resulting scattering profiles.

Membranes for Clean Water: Developing a Cure for Chlorine Degradation

Kari McPartland

Water is necessary for all living processes, from household and industry use to providing irrigation and electricity to our developing planet. Only 2.5% of the world's total water is fresh, and less than 1% of that is accessible for human use. In desert coastal metropolises from Dubai, UAE to Perth, AUS, there are already desalination factories to alleviate freshwater shortages. Currently, a high pressure process called reverse osmosis (RO) is used to purify salt water (>2000ppm NaCl) into drinking water (<20ppm NaCl) by forcing water to diffuse through environmentally-friendly polyamide-based membranes while trapping the salt ions. However, the first step to reclaiming seawater is to remove biocontaminants by chlorination. Although this treatment inexpensively prevents membrane biofouling, it also damages the chlorine-sensitive polyamide active layer ultimately causing membrane performance to suffer.

The goal of this project is to define the relationship between the performance and structure of the membrane after chlorine exposure. Specifically, the water flux across a membrane (J_w) is related to the product of the diffusion coefficient of water (D_w) and the water content in the membrane (ϕ_w). Water flux as well as salt rejection by the RO membrane can be characterized experimentally using a pressure cell method called Deadend Water Filtration (DWF). A Quartz Crystal Microbalance (QCM) was used to calculate D_w and measure mass uptake due to swelling because it can sense the slight mass increase as water is adsorbed by the membrane, which correlates the changes in the polymer structure to the performance degradation caused by chlorine. From a polymer structure perspective, chlorine ions break down the membrane by oxidizing the polyamide crosslinks and loosening the network. The loosening of the polymer network also causes the membrane to swell more, increasing the diffusion coefficient, mass uptake, and thus water content. This structural change weakens membrane performance by letting through more water and salt ions, i.e. increasing water flux and decreasing salt rejection. We found that although the chlorine has an effect on the RO membrane, it is more complicated than it first appears. Longer chlorination times lead to decreased water flux, confirmed by a smaller D_w. The salt rejection is also definitely compromised, dropping from highs of 88% to as low as 15% after 175 hours of chlorination.

Electrochemical Deposition of Pt_3Ni Ultrathin Film Catalysts for PEM Fuel Cells

Eshwari Murty

A polymer electrolyte membrane (PEM) fuel cell is an electrochemical device of great interest to the automobile industry. To attain high energy conversion efficiency, PEM fuel cells need a significant amount of Pt-based catalysts to render fast chemical reaction kinetics. Finding ways to maximize Pt utilization has been a recurring research theme over the last two decades. Catalysts whose outmost surface consists of a Pt monolayer are especially appealing.

Our group recently developed and reported on a novel electrochemical deposition method for fabricating such low-cost Pt-monolayer catalysts. It was a self-terminating process by which Pt deposition was quenched upon growing a monolayer in spite of the deposition overpotential being in excess of 1 volt. The quenching was attributed to the alteration of the double-layer structure induced by formation of a saturated H adlayer, which prevented the adsorption and reduction of Pt complexes. In this work, the former hypothesis was systematically tested. By introducing and varying the Ni(II) concentration, the self-termination was lifted as the H adlayer was disrupted by the presence of Ni on the Pt surface. The dependence of Pt deposition kinetics on Ni(II) concentration was carefully examined using electro-analytical techniques. X-ray photoelectron spectroscopy (XPS) studies were conducted to determine the composition of Pt overlayers for films prepared under varying conditions (i.e., deposition time and Ni concentration), as well as to derive the film thickness. The surface morphology of deposited films was obtained using scanning electron microscopy (SEM). After exploring a wide range of deposition conditions, we developed a protocol for growing Pt_3Ni films of 2-3 monolayers thick, a catalyst with the same composition has shown the highest activity to date for oxygen reduction reaction (ORR) in PEM fuel cells. Our ongoing work will be focused on characterizing the performance of our newly developed catalyst.

Measuring and Modeling Parasitic Resistances in CMOS Transistors

Franklin Nouketcha

A polymer electrolyte membrane (PEM) fuel cell is an electrochemical device of great interest to the automobile industry. To attain high energy conversion efficiency, PEM fuel cells need a significant amount of Pt-based catalysts to render fast chemical reaction kinetics. Finding ways to maximize Pt utilization has been a recurring research theme over the last two decades. Catalysts whose outmost surface consists of a Pt monolayer are especially appealing.

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The Impact of Robot-Human Collaboration

Tom Oeste

Over the last fifteen years, the movement of manufacturing to countries featuring labor with low hourly wages has motivated the development of a new generation of industrial robots that can work side-by-side with human workers. This technology, Human-Collaboration-Robotics, combines the intelligence and dexterity of humans with the strength, repeatability and endurance of industrial robots. Robots, however, are powerful moving machines, and the safety of humans working around these robots has become a top priority for safety standards development. We are using bio-simulant materials for the construction of disposable Human-Collaboration-Robotics safety testing artifacts, which will make possible the measurement of forces and strains when humans and robots come into contact and the severity of injuries caused by robot static and impact pressure.

To test and calibrate these artifacts we have constructed a Dynamic Impact Testing and Calibration Instrument (DITCI), which measures the acceleration and force of the impact event between a metal tip and a skin bio-simulant artifact, recording the measurements through a LabVIEW application. Over the course of the summer, we developed this application to acquire measurement data, perform numerical analysis, graphically display the analyzed data, and fit material parameters to the data to determine the viscosity and stiffness of the skin bio-simulant. Before data acquisition, the user can change the acquisition rate and time, as well as easily enter sensor-specific calibration information, so that the measurements taken are as accurate as possible. During data analysis, the user can change signal filtering parameters and graphically view various combinations of data (collected force and acceleration, along with calculated velocity and displacement) in order to better understand the nature of the impact event. Finally, the user is able to select from several parameter-fitting methods, ranging from a linear least squares fit to a transfer-function-based curve fitting. In this way, we hope to increase the legitimacy of the resulting parameters, and thus increase the legitimacy of the DITCI itself. With a well-calibrated instrument and robust analysis techniques, we hope to advance the field of Human-Collaboration-Robotics by ensuring the safety of the human workers involved.

Improving Emergency Evacuation Effectiveness
Hidemi Omori

How do we know if emergency messages are effective enough to stimulate timely and efficient building evacuations? Confusing or unreliable messages, whether textual, visual, audible, etc. have been known to discourage occupants from evacuating during emergencies, which may result in injury or death. The purpose of this project is to provide guidance, standards, and testing methods that can improve the effectiveness of emergency messages. Therefore, in this project, I worked on a literature review on how to compose, format, and test emergency messages for greater efficiency. Emergency message writers can follow the Federal Plain Language Guidelines for guidance on writing for the audience, message organization, sentence structure, etc. In addition, Message Maps and the "3 & 30 Principle" identify the concept of writing message in three sentences with less than 30 words for successful message formatting. This review also provides paraphrase, usability, and readability test methods that can improve message effectiveness.

As an additional project, building egress systems are designed with little consideration of occupant behavior, needs of emergency responders, and evolving technologies. Newer building designs such as skyscrapers demand more efficient egress systems beyond the traditional stairwell method in order for safer evacuations. The purpose of this project is to understand how high-rise buildings around the world incorporate elevators into their evacuation procedures. To collect data on evacuation procedures of tall buildings, I spoke with building management personnel from the Shanghai World Financial Center and Taipei 101, as well as compiled research findings on evacuation procedures or other skyscrapers (including the Petronas Twin Towers, Burj Khalifa, and Abu Dhabi Sky Tower). The Canary Wharf financial district in London, UK uses elevators as a means for evacuation during Imminent Catastrophic Events. Taipei 101 in Taiwan utilizes refuge areas, trained staff members, and firefighter elevators as part of their emergency evacuation procedures. In this presentation, I will present my findings on elevator evacuation procedures from 6 buildings around the world in order to improve egress system design for tall buildings in the United States and around the world.

Engineering Polymer Fiber 3D Composite Scaffolds for Enhanced Periodontal Tissue Regeneration
Charles Onyenemezu

Periodontal disease is a chronic inflammatory condition that can potentially lead to tooth loss when connective tissue attachment in periodontium is severely damaged. In order to regenerate the lost periodontal structures, a technique called guided tissue regeneration is often applied. This periodontal regenerative therapy utilizes patient or donor bone grafts that are packed into a defect site and covered with a biocompatible membrane. In this procedure, a piece of mesh-like material, the membrane, is inserted between the tooth and gingival tissue to allow regrowth of the periodontium. This mesh must function diversely: initially as an area to attract various cells then facilitate cell proliferation and differentiation and finally to form functional tissue. Obtaining necessary multi-functionality of the membrane is challenging and requires proper material design to balance scaffold's morphological and chemical properties and biodegradation rates.

In this research project an airbrushing technique was applied to fabricate 3D polymer scaffolds with diverse chemical composition and controlled average pore size (18-36 µm). The airbrush technique allows for rapid film formation from various polymers and their blends in benign organic solvents. Specifically, polymer composite fibers were synthesized by mixing poly-DL-lactide (PDLLA) with lower molecular weight carboxylic or ester group capped PDLLA polymers. Hydrophilic polyethylene glycol (PEG) polymer, Mg/Al ion rich polylactic acid and amorphous calcium phosphate compounds were also investigated for their effect on scaffold biodegradation rates. The synthesized materials were further characterized by measuring water contact angle, analyzing scanning electron microscopy (SEM) images and tested in cell culture condition to assess extend of cell penetration.

The results established that controllable biodegradation can be achieved by varying polymer chemical composition. In a comparative look at chemical composition, polyethylene glycol (PEG) polymer film demonstrated a high affinity for water when compared to other films. Additionally, a direct correlation between pore size and cell penetrative ability confirmed a deeper penetration within polymer films of larger pore size.

Measuring the Power Supply of the Future

Emily Ruppel

The only tool available to achieve "Wide Area Measurement Protection and Control" (WAMPAC) of the power grid is the phasor measurement unit (PMU). A PMU provides real time measurements that have a variety of applications in power system analysis. Data from PMU's placed strategically throughout the grid is often called upon in the aftermath of system failures to quickly assess the causes, but it can also be used to provide system operators with an understanding of the normal behavior of a large sector of the power grid.

In order to implement a system of PMU's it is necessary to determine the levels of measurement accuracy to which they can all be held under different signal conditions. The IEEE "Standard for Synchrophasor Measurements for Power Systems" (IEEE Std. C37.118.1-2011) sets the error limits for PMU's and includes an informative annex that describes a reference signal-processing model.

Though the model has been tested extensively in the process of setting standards for PMU's, it has only been tested using purely digital waveforms. The focus of this project is to instead test the PMU model using real signals generated according to the test condition requirements outlined in the standard. The effect of quantization error and distortion from the analog to digital signal converter on the model's performance can then be determined and used to evaluate the achievability of the error limits set forth in the IEEE standard (IEEE Std. C37.118.1-2011) as well as a proposed amendment (PC37.118.1a).

In Situ Characterization of Polymer Adsorption Properties Using Quartz Crystal Microbalance

DoRonne Shyu

There is a fundamental need to accurately characterize distributions in macromolecule structure, size, and chemical composition, which results in different thermodynamic and rheological properties of the material. By quantifying and characterizing polymer interactions at a model stationary phase, the understanding of polymer separation phenomena can be further investigated. This is especially important in polymer-modified surfaces where the surface is responsive to reaction conditions, such as solvent quality and temperature. In order to synthesize the stimuli responsive platform, a quartz crystal microbalance with dissipation monitoring (QCM-D) was used to characterize polymer brush formation in real time, while observing mass and mechanical property changes to the adsorbed layer. The studied polymer system consisted of tethered amine-functionalized polystyrene brushes in solvents (cyclohexane, methanol, toluene), and in the presence of poly(methyl methacrylate). QCM-D can also be used to quantitatively determine polymer chain conformation in solvent environments of varying quality. The brushes were exposed to differing ratios of toluene (a good solvent) and methanol (a poor solvent), and then to dilute solutions of free poly(methyl methacrylate) chains in identical solvent ratios. This project aims to understand and quantify the effect of solvent quality on polymer brush conformation and the resulting effect of brush conformation on free polymer adsorption to the brush. Ultimately, this project will help develop quantifiable methods for the next generation of stationary phases used in polymer separations.

Virtual Calibration: Using an iPhone to Calibrate Multiple Microscopes

Jacob Siegel

How would we build an inexpensive array of handheld microscopes for measuring microscopic dynamic events over a large field of view? The challenges of building such an instrument lie in estimating spatial, temporal, and color properties of each handheld microscope, as well as in integrating and extrapolating individual non-overlapping fields of views into a large field view. To address the above challenges, we assembled first a linear array of four digital handheld microscopes (USB cameras). These microscopes are currently used primarily for skin and scalp dermatology and printed circuit board inspection. Next, we developed calibration methods to perform pixel-to-millimeter conversion, red-green-blue color normalization, and microscope pose estimation using a high-resolution liquid crystal display (LCD) of an iPhone. The iPhone LCD renders temporally varying pixel intensities of a web page content that represents a dynamic virtual calibration object. The current virtual calibration objects consist of moving lines in two orthogonal directions with known line spacing and motion vectors. Our custom-developed software processes the LCD renderings captured by each microscope to determine the calibration parameters. The new calibration method is compared against the more traditional calibration methods using a physical object (i.e., a ruler for pixel-to-millimeter conversion, Gretag Mcbeth color chart, and a set of a priori known shapes and their locations for pose estimation). Our preliminary results indicate that the virtual object-based calibration is more accurate than the physical object-based calibration. In the future, we plan to investigate the dependency of the virtual object rendering on the display properties of a mobile device, and to acquire real video streams to study live cells and insect behavior.

Controlled Optical Levitation of Small Particles

George Sineriz

The discovery that optical forces from a laser light source can move particles micro or nanometers in size has led to many applications. One application is the optical levitation of small particles by counteracting gravitational forces with the radiation pressure exerted by a laser. Although this levitation can be accomplished, the position of the particle is unstable and limits the sensitivity of measurements. A combination of laser intensity fluctuations, mechanical vibrations, and other sources of noise introduced by electronics in the system superimpose fluctuations that contribute to the particle's instability. Since many useful measurements can be obtained through optical levitation it is of interest to stabilize the particle about a null set point, the deviations from which can be measured with high sensitivity. Measurements of the particle size, the radiation scattering force, wavelength dependence of the scattering force, and even accelerometer applications are possible.

An approach used to stabilize the particle about a null set point is to develop a control system that will vary the intensity of the laser to counter the fluctuations of the position of the particle in the axial position. The position of the particle will be detected with a quadrant photo detector (QPD) and will be used in a control circuit to modulate the laser intensity though an electro-optic modulator (EOM). Once the particle is stabilized with the use of this system, the various measurements defined can be performed and recorded.

Measurements of a Copper Polypeptide Solar Fuels Catalyst
Ekaterina Tolstaya

Recent advances in energy research exploit catalysts composed of peptides and metal ions to create new nanomaterials for converting water to hydrogen. A highly stable copper (II) polypeptide complex has been shown to electrocatalyze water oxidation, but questions remain about the water oxidation mechanism. In particular, the key intermediate species contains Cu^{4+}, an oxidation state that is rare for copper. Our goal is to generate and trap this Cu^{4+} species. The catalytic and spectroscopic properties of the complex were investigated using techniques amenable to aqueous solution measurements: electronic absorbance and electron paramagnetic resonance (EPR) spectroscopy. Following a 20 second lag phase, we observed slow formation of a species by visible absorption spectroelectrochemistry, which we tentatively assign to the (hydro)peroxide intermediate proposed by Zhang, et al. (Zhang et al. *J. Am. Chem. Soc.* (2013), **135**, 2048). In situ trapping and detection of the high-valent Cu^{4+} species by EPR-based spectroelectrochemistry is underway. The system of measurements being developed and conducted can be used to characterize a variety of other catalysts, including catalytic metal sites on nanostructured biomaterials.

Evaluating a Machine Learning Algorithm for Span Detection Through Standardizing Spam Characterization
Mark Villarrubia

Web spam is unwanted advertising, marketing, or malicious content on the web. The goal of the spammer is to get the user to buy a product, to click on a link to create advertising revenue, or to download malware. Spammers employ a variety of strategies to disguise spam as real content, to encourage legitimate web sites to link to it, or to get search engines to display it to users. Methods for automatically detecting and removing web spam improve the quality of the web by making good content easier to access.

This project has two goals. First, we need a set of guidelines that people can use to identify web spam consistently; no such guide currently exists. Second, we need a large set of examples of spam and non-spam web pages to train an automatic spam detector. We label a large volume of spam and non-spam web pages, documenting the rating process in order to provide a standardized procedure for later assessors. With this example data, we train an algorithm to distinguish spam from non-spam, and run it using part of the example data as training and part as input to be classified, in order to measure the accuracy of the training algorithm.

We drew a random sample of web pages from ClueWeb12, a collection of 800 million web pages built by CMU for web researchers. We first developed human guidelines for identifying web spam consistently. We then labeled the remainder of the sample following the guidelines. Finally, we used the labeled data to train a logistic regression classifier to identify spam automatically, and evaluated its accuracy. This classifier will be integrated into a search engine used here at NIST for building web datasets.

Design and Construction of a Differential Current Amplifier for Capacitance Measurement with an Atomic Force Microscope Probe

Benjamin Walsh

As improvements in integrated circuit fabrication technology continue to reduce device size, increasingly smaller characteristic capacitances can limit speed. Explicit knowledge of these and other parasitic capacitances in the sub-femtofarad range are necessary for robust modeling in computer aided design. Yet conventional commercial meters that measure capacitance introduce stray capacitances often orders of magnitudes larger than the target capacitance. Charge-based capacitance measurement (CBCM) has been introduced to measure small interconnect capacitances, and has been modified to characterize non-linear MOS capacitors. CBCM extracts capacitance from measuring average DC current, and can subtract parasitic capacitance of the transistors connected to the target capacitance. C-V curves were extracted for a test chip containing MOS capacitors of different sizes using modified CBCM to verify design viability. Experimental results compared well with theory, and critically were consistent within ~50aF. To reduce stray capacitances when measuring, such as those associated with a pad, probe, and cable, modified CBCM was then implemented on a printed circuit board (PCB) to interface with an atomic force microscope (AFM) probe. To facilitate high SNR in current measurement, several current differential amplifiers were simulated before choosing a final design. The final PCB, which includes modified CBCM and the chosen current differential amplifier, was designed to interface with AFM and measure the capacitance of nanostructures with attofarad resolution.

Improving Quantitative Immunostaining Measurements by Atomic Force Microscopy

Grace Wang

Properties of gold nanoparticles (AuNPs) such as an inert, stable gold core and controlled cellular uptake make them possible non-toxic carriers for target-specific drug delivery. Their role in nanomedicine drugs makes consistency in the surface coating of nanoparticles important in drug development. Thus, measurements with single particle fidelity must be developed in order to better understand how substances bind to the particles. An approach for determining the upper limit of detection will be presented. Quantitative immunostaining is an antibody-mediated self-limiting self-assembly approach for measuring low surface-density molecular coatings. The conjugation of probe (10 nm diameter) nanoparticles to analyte (60 nm diameter) nanoparticles through quantitative immunostaining is informative on the orientation of their binding and the overall surface heterogeneity as observed by atomic force microscopy (AFM). The impact of monoclonal versus polyclonal antibodies was studied on analyte nanoparticles with varying ligand ratios; the probe to analyte ratio is then observed and quantitatively analyzed by predictive models that assume random orientational deposition and compensate for AFM being a topographical observation. AFM sample preparation methods must ensure that nearly all probe to analyte ratios observed for a control of unsynthesized, unconjugated probe and analyte particles are 0:1; the impact of such variables in synthesized and conjugated probe and analyte particles were clearly observed.

Analysis of Stairwell Evacuation

Emily Wiess

In response to the tragedy caused by the 2001 World Trade Center attacks, NIST began collecting evacuation data from high-rise buildings with the goal to mitigate the amount of lives lost due to inefficient egress designs and procedures. NIST observed 14 full building evacuations of all occupant types, including those who were mobility-impaired. Analysis of this data will provide a more comprehensive quantification of evacuee movement and explanation of human behavior, which will strengthen the validity and predictive capability of current egress models. The performance based-design of buildings involves a direct comparison between the ASET (available safe egress time) and RSET (required safe egress time) components. NIST focuses on the time occupants need to complete a safe evacuation by performing analytical calculations of certain variables such as: pre-evacuation delay, total clearance time, overall speed, and peak density.

Utilizing Microfluidic Platforms to Develop Microbial Pathogen Separation Techniques

Rebecca Zubajlo

At the moment, there is no method to rapidly detect low concentrations of microbes in a complex sample such as soil, water, and food. Food and water contamination is a major problem, according to the Center for Disease Control, with 12 outbreaks of *Salmonella* in 2012 and 3 of *Escherichia coli (E. coli)* in the United States alone.[1 2] This results in 265,000 pathogenic *E. coli* infections in the United States per year.[3] Current methods to separate and detect bacterial contamination in samples use centrifugal force or magnetic and electric field separation techniques that require amplification and processing of the sample prior to detection.

However, bacteria have a unique ability to interpret the world around them. Bacteria are capable of sensing chemical and physical signals from the environment and responding rapidly. The focus of this study was to use these biological properties to separate *E. coli* and *Salmonella* into two distinct populations with low initial concentrations of the bacteria in a complex sample.

To achieve maximum separation of the bacteria, the chemotactic properties of *Salmonella* and different strains of *E. coli* were tested using various chemicals. The separation of the bacteria was quantified using a series of time-lapsed microscope images of the chemical mixed with green fluorescent protein and the concentration of cells across the microfluidic channel.

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[1] http://www.cdc.gov/salmonella/outbreaks.html
[2] http://www.cdc.gov/ecoli/outbreaks.html
[3] http://www.cdc.gov/ecoli/general/index.html#who-

University of Missouri Kansas City

How to Blow a House Down: Confessions of the Big Bad Wolf

Jason Regina

High winds cause the largest losses due to natural disasters in the U.S. In hurricanes alone, annual losses due predominantly to high winds averaged on the order of $10 billion from 1990-1995. Low-rise buildings such as single-family residences and small commercial structures, which constitute over 70 % of the U.S. building stock, account for the majority of these losses. Accurate prediction of wind-induced loads on low-rise buildings has proven difficult due to the complexities involved in modeling the portion of the atmospheric boundary layer (ABL) in which these buildings reside. As the lowest portion of the atmosphere, flow in the ABL is highly turbulent due to the influence of the Earth’s surface. Wind tunnels that simulate the ABL have previously been used to estimate the expected wind-load on low-rise buildings. However, the lack of a standard for generating the turbulent flow that characterizes the ABL has resulted in significant variation among estimates.

This study began modifications to a high-speed wind tunnel, used primarily for calibration of anemometers, to an ABL wind tunnel for estimating wind-loads on structures. Preparation for this research included instrument calibration and validation of system configuration, such as probe placement and sampling frequency. Initial data acquisition and processing was performed to develop routines that produced basic wind flow characteristics of an empty tunnel. The routines developed to characterize the empty wind tunnel were used to test the incremental installation of various roughness elements used to model the ABL.

University of Puerto Rico

Neutron Diffraction Study of Pressure-Dependent Magnetism in Molecule-Based Magnets
Steven Conklin

Pressure dependent magnetism in metallic alloys is useful in sensors, and one application is sonar detection by the military. Recently, molecule based magnets (MBMs) are emerging as a possible alternative to the existing technology, with the added benefit of room-temperature synthesis that is highly tunable giving the ability to engineer systems with multiple functional properties. A promising group of MBMs are the Prussian blue analogues (PBAs), which are part of a select group of bimetallic cyanides in which magnetic ordering can be tuned by external stimuli such as light, electric field, and pressure. Two PBAs that display pressure sensitive magnetization are $KFe_3[Cr(CN)_6]_2$ (Fe-Cr) and $KNi_3[Cr(CN)_6]_2$ (Ni-Cr), and there are open questions about the details of the observed effects. Presently, it is believed that under applied pressure, Fe-Cr undergoes a linkage isomerism (LI) that changes carbon coordination of the CN from Cr to Fe, resulting in a change in magnetic configuration of the Fe cation from high-spin (HS) S = 4 to low-spin (LS) S = 0, thus reducing the observed magnetization. On the other hand, Ni-Cr is thought to undergo random spin-canting due to bond-deformation or LI. We utilize neutron diffraction (ND) to test these theories. For Fe-Cr, ND has the power to observe the LI effect, since ND, unlike x-ray diffraction (XRD), is similarly sensitive to transition metals and organic elements. For the Ni-Cr system, we will also look for LI, as well as random-spin canting from the magnetic interaction of the neutron with the system. Polarized beam experiments are also performed to test a contrary hypothesis of domain wall movement in Ni-Cr providing the pressure sensitive magnetism. Supporting probes Fourier transition infrared spectroscopy (FT-IR), XRD, and x-ray photoemission spectroscopy (XPS), are used to further characterize the samples. Preliminary results suggest no LI in either sample and domains as the primary effect in Ni-Cr.

Measuring Software Performance on Mobile Devices
Ramón DeJesús

The goals of this project are to replace unreliable benchmarking practices with rigorously-studied methods grounded in design of experiments and to solve measurement challenges created by the evolution and increased complexity of commodity hardware.

On desktop machines where CPU time benchmarks trace to hardware cycle counters in the CPU, we have found such variability that the naive approach of running a benchmark a few times and averaging the results is not trustworthy. Similarly, when profiling the call tree of applications, we easily found examples of incorrect results from commonly used tools. The task for the summer is to investigate the same problem area for one or more mobile platforms to see if the same or similar problems exist and what must be done to get good performance measurements.

Focusing on the Android OS, a series of tools is being developed this summer to achieve these kinds of measurements. When applying a new tool in a new environment, we need first to validate the tool to know that it gives accurate results. For this purpose, an existing validation suite was ported to Android/Java to validate results from the Dalvik Debug class. However, significant findings require a lot of data collection. To make things easier in the mobile environment, a test driver and scripts were developed to automate this gathering process.

In the long run, we'll be proceeding to use and adapt these products to different performance measuring tools and different experiments. By the end of the summer we expect to have significant findings about performance measurement in this new and rising environment.

Manufacturing Sensor Knowledge Representation

Kevin Molina Serrano

My research project consists of building a knowledge representation (an ontology) focusing on the manufacturing sensor capabilities and characteristics by adding the manufacturing sensor requirements to the SSN Ontology (Semantic Sensor Network Ontology). This manufacturing perception sensor ontology will be used to provide a basis for measurement techniques to evaluate system performance, support design of sensor networks for manufacturing applications, categorize and organize calibration techniques for sensors and sensor networks, reason about available sensors and capabilities to meet during operation, create mechanisms and languages for querying sensors and provide logs and data provenance for potential legal and regulatory review. Some of my tasks were to review the SSN Ontology and some manufacturing scenarios and use these scenarios to better understand and model the requirements of the manufacturing sensor ontology. Some of the requirements that were added to the SSN Ontology were classes like actions, domains, robot components, and states, among others. The SSN ontology is represented in the Web Ontology Language (OWL), and extension to the ontology were made in this language. Finally, we came up with the first draft of the manufacturing sensor ontology and in the future, it will be used as a standard for the requirements of the sensors in the area of manufacturing.

Density of States Characterization in Single Crystals of Rubrene

Michael Morales-Otero

Organic electronics is a revolutionary research field. Semiconducting organic materials have certain advantages over inorganic materials such as low cost and flexibility. These properties make them ideal for the development of devices such as organic LEDs, transistors, flexible displays and solar cells. This study focuses on charge transport in organic single crystals of rubrene. The uniform composition and structure make it possible to identify the fundamental limitations to the transport of electric charge. Of special interest to us is the distribution of trap states in intrinsic rubrene because the performance of organic semiconductor devices is often determined by their specific trap distributions. Among organic semiconducting materials, rubrene is of special interest due to its high charge mobility. To create rubrene crystals we employ a temperature gradient crystal growth furnace. Using a flow of argon and a temperature gradient, the rubrene is sublimed in the furnace, transported along the length, and deposited, forming crystals where the lower temperature is ideal for growth.

The objectives of this research are to grow single crystals of rubrene using the method of physical vapor transport, identifying the ideal parameters for crystal growth. Single crystals are laminated onto Field-Effect Transistors (FET) test beds and their field-effect mobility is measured. The distribution of trap states in rubrene single crystals is measured using temperature -dependent space charge limited current (SCLC).

WiFi Indoor Localization

Manuel Ortiz

Commercial or governmental applications that are accessible and affordable to target indoor localization are not available. There are plenty of outdoor localization methods like GPS (Global Positioning System), which is used for many purposes and solves many localization needs.

WiFi technology can be used to solve the problem of indoor localization, since there is a wireless card in any computer-like device; it is the most affordable method for localization that can be developed without incurring excessive costs of equipment.

This project deals with localizing persons or objects equipped with a WiFi radio inside a building. The process is based on taking WiFi fingerprints in specific points in the building. A WiFi fingerprint is a scan of the WiFi signals received at a particular point. Specifically, it consists of the (x,y,z) localization of the point, the MAC addresses of the WiFi, Access Points (APs) found, and the strengths of the received signals. Later when the objector person performs a WiFi scan, the received signal strengths can be compared with WiFi fingerprints available, and the location to the “closest” fingerprint declared as an estimate of the location of the target or person to be localized. This project is being tested with Android cell phones. An application has been developed to perform the WiFi scans in the Android system and store the data. The application is also able to analyze the data and provide an estimate of the localization depending on the map that it has from the fingerprints.

The project demonstrates how WiFi can be used to find the localization inside a building in the most accurate way.

Collection of Standard Reference Data for Gas Adsorption via Molecular Simulation and Literature Meta-Analysis

Jaime Santillan

In the 19th century, scientists realized that gases play a crucial role on Earth’s energy balance. The heat that is trapped by the greenhouse gases keep us warm enough for sustaining life. But massive release of major greenhouse gases carbon dioxide and methane, as consequence of anthropogenic activities, have been increasing the average temperature of the planet for many years, producing a climate change. So a global approach is in process to mitigate that emission of gases, developing new adsorbent materials with high storage capacity and excellent adsorption selectivity. Despite advances in material development, standard reference data with well-defined features of adsorption isotherms are presently insufficient and represent a challenge to designing novel adsorbent materials that are chemically stable and easy to regenerate with minimal energy input and easy to synthesize [1].

Recently, a computational approach has been developed to rank adsorbents according to their performance in carbon capture and storage [2]. Molecular simulation has been used to predict the adsorption isotherms and to enable screening of metal organic frameworks in a high-throughput manner. In addition, reference data for Argon adsorption [3] is suitable for calculating surface area, micropore volume, and pore size characteristics of sample materials as part of understanding novel designs.

By the above, development of Standard Reference Data is quite important, because one of NIST's missions is to help industry to improve products and services. As a National Laboratory, NIST has the vital challenge to establish standard reference materials and data that verify research and substantially aid future materials development.

We conducted molecular simulation of Argon adsorption on graphitic carbon and carbon nanotubes to collect information for standard reference gas adsorption isotherms. Transition Matrix Monte Carlo (GC-TMMC) [4] was used as a demonstration of its ability to be a standard tool for simulating gas adsorption processes on carbonaceous materials. This method generated multiple adsorption isotherms from probability distributions generated by simulations from which we identify coexisting phases. Further work has collected experimental gas adsorption isotherms from the scientific literature which allows for meta-analysis and virtual Round-Robin comparison of adsorption measurements.

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University of South Alabama

Sustainable Thinking in the Design Environment
Haley Hill

In the design environment, Life Cycle Analysis (LCA) tools are being used alongside Computer Aided Design (CAD) tools to assess the cradle-to-grave sustainability implications of products to be manufactured. To support sustainable thinking in Computer-Aided technologies (CAx) environments, NIST researchers are developing a material information model for sustainability. Material choice significantly influences the sustainable impact of a product, from beginning to end-of-life. With improved access to material information, product designers can attain newfound insight into the sustainability implications of their design decisions. A well-constructed material information model can provide the necessary access, and therefore the desired insight.

The goal of this project was to develop a proof-of-concept implementation to highlight the benefits of such a material information model. A collaboration opportunity with Sustainable Minds, LLC, provided a platform for a proof-of-concept implementation within an LCA software tool. To gain an initial understanding of where key contributions could be made, numerous LCAs were conducted within the software. Evaluation of the procedures and the results revealed several areas where the availability of material information could foster more intuitive design-time decision making. Collaboration focused on powder metallurgy (PM) processes, for which key material properties were identified. The selected properties support the evaluation of process performance and provide users insight into sustainability implications of PM product design decisions. The methods used and results achieved will be discussed in this presentation.

University of South Florida

SI Traceable Calibration of Thermal Cantilever Vibrations in a LDV
Laura Byrnes-Blanco

Atomic force microscopy (AFM) utilizes micro-fabricated cantilevers to measure materials' physical and mechanical properties. The manufacture of these cantilevers introduces variability in both dimensional and material properties in the cantilevers. It is these variations that cause the cantilever spring constants to be commonly specified with $\pm 50\%$ accuracy. Because the accuracy of an AFM's nanomechanical property data is dependent on the accuracy of the cantilevers' spring constants, it is imperative to determine the spring constant values as definitely as possible. In order to promote accurate nanomechanical property measurements, NIST is developing reference cantilevers with highly accurate spring constants that AFM users can purchase and test their commercial cantilevers against, allowing for accurate determination of commercial cantilever spring constants. We are utilizing a Laser Doppler Vibrometer (LDV) to certify the reference cantilevers and, therefore, we must calibrate the LDV in an SI-traceable manner.

To accomplish SI-traceability, our LDV is calibrated with a homodyne interferometer. Homodynes are programmed to emit known wavelengths of light and, as such, are SI-traceable. Both the LDV and homodyne systems take displacement measurements of cantilevers that resonate at a natural frequency in room temperature or from a driven frequency provided from a voltage to displacement transducer. Once this displacement data is collected (from both systems) and transformed into comparable forms (by applying Fast Fourier Transforms and instrument sensitivity values), they can be plotted against each other for similarity and accuracy determination. If these comparisons are within a certain margin of error, the LDV can be considered calibrated to the SI and the certification of reference cantilevers' spring constants can be completed.

University of Texas Austin

Automating Tunnel Junction Device Fabrication
Gabriel Jaffe

This summer I designed and built the control box for a substrate positioning system in a thin film electronics fabrication chamber. The control box powers rotational stepper motors and handles the logic to switch between computer and manual control of each motor. A limit switch system defined "end of travel limits" on the position and rotational orientation of the substrate in the chamber. I wrote a Labview program to control the temperature of the substrate as well as automatically control each motor via ASCII serial commands sent to the motor control box. The thin film tunnel junction devices created in this chamber utilize the spin properties of electrons as well as electron charge through the tunnel magnetoresistance effect. A similar effect is used in read heads for magnetic disk recorders. The goal for automating the deposition chamber is to be able to quickly fabricate devices of different configurations and compositions. My Labview program will be a small part in a larger program, which will accept "recipes" for devices as inputs, and then automatically fabricate devices to the input specifications. As devices exploiting electron spin make their way into industry and commercial use, the head of my project Dr. Josh Pomeroy will use the spin-devices created here at NIST to set a standard for measuring and manipulation electron spin.

Neutron Vision
Devin O'Kelly

Neutron imaging picks up the slack from other imaging methods. While X-rays easily pierce through water and are stopped by dense materials, neutrons have a very different behavior. Steel and titanium are highly transparent to neutrons while water and hydrocarbons are practically opaque, giving neutrons a very complementary view of materials relative to x-rays. In particular, we used it to image the enhanced oil recovery from saturated sandstone using supercritical CO_2.

The extraction of oil using supercritical CO_2 is already in place, but it was decided that an investigation into the efficiency and dynamics of the process was necessary. Ordinarily, CO_2 is injected into oil reservoirs at high temperature and pressure, thus providing the conditions for supercriticality. This serves a dual purpose: The first, that oil recovery using this supercritical fluid is more efficient than with water, and the second, that this is a potential method for CO_2 sequestration. The process of extraction was visualized using neutron radiography and tomography was performed afterwards to determine the 3D distribution of leftover oil.

In this talk, we address the use of neutron imaging in a variety of contexts, including safety investigations, the hydrogen economy, with a heavy focus on enhanced oil recovery.

<u>University of Texas Dallas</u>

Investigation of Stability of Silica Particles in Lutidine/Water Solvent
Katherine Borner

Colloidal stability is important for many industrial applications. When colloidal particles are dissolved in a binary liquid consisting of two different types of small molecules, the solution stability can be affected when approaching the phase separation temperature of the two different solvent molecules where the density fluctuation of solvent molecules becomes very large. The current project focuses on understanding how the density fluctuation of solvent molecules affects the silica particles' stability using combined experimental techniques including dynamic light scattering and small angle neutron scattering. Silica particles at different concentrations are dissolved in the solvent consisting of lutidine and water at different ratios. We utilize ultraviolet-visible spectroscopy and dynamic light scattering to probe the cloudy point temperature of the solutions at which the "critical opalescence" occurs. The phase diagrams of the silica particles in lutidine and water mixture solvent are thus determined. We then use small angle neutron scattering to measure the scattering patterns of the silica particles in the one phase region from which the interaction between the silica particles will be determined. We are also interested in the possible chemical reaction between the silica particles and the solvent at different temperatures that may affect the long term storage capabilities of the silica/water/lutidine solutions.

<u>University of Virginia</u>

Requirements Analyses to Support a Material Information Model for Sustainability
Aarvind Harinder

Materials, and therefore material selection, influence the sustainable impact of a product from beginning to end-of-life. Improved access to material information can provide designers with the necessary insight into the sustainability implications / tradeoffs of their design decisions. Insight into lifecycle tradeoffs requires access to both upstream and downstream information at design time. This access can be facilitated by information transparency between information representations across the life cycle. A well-constructed Material Information Model (MIM) can provide the necessary access, and therefore the desired insight.

Researchers at NIST have developed a set of requirements that a MIM for sustainability must support to provide the desired design-time information access. Using these requirements as guidelines, I analyze several information representations (ANSI/ISA 95, BPMN, ISO 10303, ISO 15926, MatML, SCOR, and SysML) currently available for information management at various stages of the lifecycle. I compare and contrast the extent to which these representations meet the information needs of the MIM. I assess the level to which information synthesis may be achieved given the varying degrees to which the MIM requirements are met. I then take a step forward and demonstrate how each representation can be used to model sustainability-related information and the extent to which MIM requirements are satisfied. Finally, I will introduce where synthesis challenges lie and the steps required to overcome them.

Developing Ontologies Through a Root-Based Vocabulary In a Semantics Database

Alexander Yang

Current challenges involving big data include the integration of information. Given the vast quantity and federated nature of information, data is inaccessible and searching is inaccurate. As a result, scientists and engineers encounter difficulty in obtaining data relevant to their studies. Typical searching techniques are vague and indiscriminate to the use cases and customized requirements of the user. Normal vocabulary is vague and cannot distinguish based on context. Its utilization in search queries leads to mixed results and misreads that need clarification from the user. Furthermore, information and data are not organized or clustered together to catalog research in a top-down manner, hindering the ability to view connections between research documents. However, the implementation of semantics connects related information and increases overall accessibility.

As an extension of the brain mapping initiative, materials genome initiative, and open government projects, we developed a technique to annotate documents using a high-value, root-based vocabulary, modeled after Sanskrit and Latin, to illustrate semantic concepts. Rules were developed to streamline the root-based vocabulary, and first ontologies were designed as knowledge structures to depict relationships among related research.

University of Washington

An Optical Force-to-Frequency Transducer

Rachel Kearns

This research aims to develop a highly precise and stable mass balance using a rigid glass piece with a built-in Fabry-Pérot optical resonator as displacement sensor. By placing a mass (of nominally 1 kg) on top of the rigid glass piece, the length of this solid will compress, which can be very accurately measured by the Fabry-Pérot laser sensor.

The Fabry-Pérot cavity consists of two mirrors quasi-monolithically attached to a cylinder of Ultra Low - ULE glass by means of hydroxide catalysis bonding. The mirror reflective surfaces are aligned towards each other and separated by a distance of approximately 0.08 m. A system has been constructed to allow a kilogram mass to be placed on top of one end of the cylinder, resulting in a compression of this solid and movement of the mirrors closer together. Due to the Young's modulus of the ULE glass (67.6 x 109 N/m2) this mass is expected to compress the cavity length by approximately 21 nm. The wavelength of a laser will be tuned to equal an integer multiple of the cavity length, thus becoming resonant. When this occurs, the amount of laser light transmitted through the cavity changes significantly. When the laser is not in resonance with the cavity, most of the light is reflected back. Optical resonance is given by the integer multiple relations between the laser wavelength and the cavity length. Measuring the intensity variations in the reflected light allows very precise monitoring of a change in cavity length caused by the compression of the cylinder due to the applied mass.

The goals of this project are in line with the NIST Watt Balance project, which has been in progress since 1980 and defines 1 kilogram to an accuracy of the order 10-8.

University of Wisconsin Platteville

A Case Study of a Turning Machine to Validate Sustainable Process Analytic Formalism

Joseph McIllree

Major manufacturing enterprises have been continuously facing demands for sustainable manufacturing to comply with enforced environmental regulations, competitiveness, and occupational safety and health. To advance sustainable manufacturing infrastructure in a factory, optimization technology is needed to help make decisions for enhancing energy or material efficiency. Recently, NIST has proposed the methodology of Sustainable Process Analytics Formalism (SPAF) that provides a mechanism to represent the knowledge of process flow, data, and mathematical specification for sustainability analysis and optimization. Based on data collection from a real and virtual machine, a case study will be performed of a turning machine process using SPAF to find optimal manufacturing parameters.

This project aims to develop a virtual machine that emulates the real turning machine (e.g., MAZAK QT 300M) in the NIST machine shop for sustainability data generation and to find the optimal manufacturing parameters (e.g., spindle speed (rpm), feedrate (m/s), and depth of cut (mm)) from the sustainable manufacturing perspective. Specifically, based on a data set (e.g., energy and coolant) from the real turning process, an analytical model will be created and emulated into the virtual machine model. In addition, we will also implement Sustainable Process Analytic Formalism (SPAF) model for sustainability performance analysis (e.g., optimization using IBM ILOG CPLEX) in the case of the turning process. We will validate the SPAF model of a turning machine in both real and virtual machine.

Vanderbilt University

Energy Optimization for Welding Operations

Theodore Russell

Where would we be without assembly processes? Assembly is the backbone of manufacturing, and at the center of that backbone are joining processes, the most prominent and common being, welding.

Of course welding is used in variety of industries and in a variety of ways. So how then, can we come up with a standard for welding processes? Private industry manufacturers all have their own processes, their own parameters, and most are probably largely unwilling to adapt or alter their methods. We must focus on standardizing something these processes all have in common, energy.

In this talk, I will introduce a series of relationships between process parameters for welding. These relationships will be added to an Energy Calculator, developed by my colleagues and I. The Energy Calculator is used to calculate energy consumption associated with various welding processes, allowing manufacturers to optimize their welding processes, thus reducing energy consumption, cost, and emissions. Also included in my talk is an in-depth explanation of the mathematical relationships of the process parameters associated with welding.

Virginia Polytechnic Institute and State University

Measurement Deviations of Additively-Manufactured Parts from Their Theoretical Models
Lindsey Bass

Additive manufacturing (AM) is rapidly gaining popularity as the technology becomes more economical and accessible. Industries are turning to AM for convenience of printing small parts that otherwise would take weeks to order. Even body parts have been printed via AM, which is advantageous when dealing with complex geometries with which subtractive manufacturing would struggle. Although AM has the potential to revolutionize industry, improvements must be made to turn the currently crude artifacts into valuable products. Evaluating process metrology and feedback control of powder-bed-based printers is a systematic way to analyze part consistency and quality. One way to investigate this is through process-intermittent measurement in which a camera mounted on the printer snaps photos for every layer. While a Labview program retrieves these images, a similar program acquires screenshots from the monitor of the theoretical images for each respective layer. A Matlab program retrieves both sets of images, converts them to binary images, properly scales them, overlaps them in the most efficient way, and measures the distances between corresponding regions. Average deviation values for each layer effectively approximate the printer's performance. Initial tests have shown deviations almost reaching 1 mm, which demonstrates the need for improvement before applying AM to products requiring higher precision. We found by monitoring the deviations, the program outputs an error if the values exceed the specified tolerance. Furthermore, continual monitoring of layer deviations can contribute to feedback control of the additive system resulting in improved part quality.

CFD Simulation of Flow Around Bluff Body Objects
Kelly Webster

Computational Fluid Dynamics (CFD) is a powerful tool for wind engineering applications with a potential to replace traditional wind tunnel testing. However, the usefulness of practical CFD calculations is limited by the difficulty of simulating the wind-induced flow around bluff bodies.

The objective of this project is to perform CFD calculations using Fire Dynamics Simulator (FDS), public domain software developed by NIST. FDS models turbulent flow using the Large Eddy Simulation (LES) method, which solves filtered Navier-Stokes equations; large eddies are solved and small eddies are modeled. The goal is to check the software's capability to simulate flow characteristics around a square cylinder in various types of incoming turbulent flow, including: the Kármán vortex shedding phenomenon, pressure distribution on the cylinder surface, and aerodynamic forces on the cylinder. The results of the calculations will be a contribution to the problem of evaluating the capability of the software to simulate wind-induced wind pressures on bluff bodies such as buildings. In order to determine the practicality of CFD calculations, data obtained from FDS is compared to experimental data from the NIST wind tunnel.

Virginia State University

Inheritance in Attribute Control Policy
Bruce Batson

Attribute Control Policy (ACP) is used to determine who can do what action, to what source, and at what time. The way ACP does this is through the use of four different attribute types. The four types are subject, action, environment, and resource. Rules are then made using these attributes. A rule will state that a subject or combination of subjects are either permitted or denied from performing an action on a resource in a certain environment. NIST has a program, known as the Attribute Control Policy Tool, which allows a user to create an Attribute Control Policy and test the rule to make sure there are no rules that conflict with each other.

My project for the summer is to add a tab in the program that allows the user to add inheritance. In ACP, inheritance is when a subject attribute gains the same permission as one or more different subject attributes. For example, say that a policy has two subject attributes named John and Jack. Jack inherits John and there is a rule that states John is permitted to read file A, and is denied from reading file B. Through inheritance, Jack is also permitted to read file A, and denied from reading file B.

With this tab added, it will be easier for a user to create rules through inheritance. Without the tab, the user had to create rules for inheritance manually. So if a policy had 30 rules about John and Jack inherits John, then the user would have to add the 30 rules that Jack inherits manually. After reading and understanding the source code for the program and researching more on how J Trees work in Java, I was able to add to the source code so that the program will automatically make rules based on inheritance.

3D Topography Analysis of 10 Consecutively Manufactured Drift Punches
Taher Kakal

In an effort to address the lack of objectivity in visual toolmark identifications, this project aims to provide mathematical validation of the scientific foundation. This research will demonstrate that even when tools are consecutively manufactured, the toolmarks they create can still be individually identified. In order to undertake the task NIST developed a toolmark rig which imparts the surface topography of the tool (punch) onto a surface in the form of an impression. In order to customize the rig for the sole purpose of creating punch marks without any double impression due to recoil effect, an anti-rebound mechanism was implemented using a uni-directional bearing and a set of gears.

A set of ten consecutively manufactured punches were used to create ten known punch impressions on non-pristine copper surfaces. A 3D disc scanning confocal microscope was used to measure the surface topography of each impression. Each punch was used to create two known marks. The identities of the punches were then randomized and hidden to create a set of twenty unknown marks. From the known matching distribution, a threshold score was established and used to identify the unknown toolmark in a blind comparison. Based on the statistical analysis of the known match and known non-match scores, all of the unknown impressed punch toolmarks were correctly identified back to the punch that created them. This study provides objective scientific support for the validity of toolmark identifications.

Digital Repository of Mathematical Formulae
Janelle Williams

We are developing a digital repository of mathematical formulae (DRMF) as a web resource. The overall concept is to format the repository as chapters of orthogonal polynomials and special functions. Each chapter contains sections and within each section displays a list of formulas and conditions. Important details about each formula are formatted in separate linked pages. The formulae details are sectioned off as: (1) the reproduced equation with conditions, (2) proof(s) of the equation, (3) discussion (including the literature) concerning the equation (including references to proofs), (4) a reference list for this equation, and (5) a see also list of associated functions. Corresponding with this web page will be a talk page where informal discussions concerning the equation are held. The see also list is determined by using special LaTeX macros for commonly used functions. The use of these macros within the markdown source of the formulae also allows for sophisticated search options within the DRMF. We base the implementation of DRMF on a standard MediaWiki installation. Beyond using the regular features of Wikis, the DRMF follows the "Active Documents Paradigm" by embedding interactivity via modules realized in the JOBAD framework. The modules created in the summer project, applicable in and beyond DRMF, include a clipboard for mathematical formulas and formula-oriented navigation to proof and talk pages. The overall success of DRMF hinges on the successful integration of MediaWiki, JOBAD, and a search engine for Mathematics, which is the final deliverable for this summer project.

Functionalized Gold Nanoparticles That Resist Protein Adsorption
Imani Wood

Au nanoparticles may have enormous potential in biomedical applications, from diagnostics and imaging to treatment modalities. However, concerns of non-specific protein adsorption on the nanoparticle surface may limit the *in vivo* usefulness of these nanoparticles unless a robust molecular-scaled coating can be developed to promote biocompatibility. Several NIST-developed molecules that self-assemble on planar Au surfaces may also be suitable for coating Au nanoparticles, enhancing their usefulness for biomedical purposes. Two compounds, a hydroxyl-terminated dithiol compound and a hydroxyl-terminated thiol compound, were used as test compounds in this study. Au nanoparticles were exposed to these compounds, and subsequently exposed to proteins such as fibrinogen and bovine serum albumin to observe whether the proteins would bind to the nanoparticles. The interactions between the functionalized gold nanoparticles and the proteins were measured using UV-visible spectroscopy.

Virginia Wesleyan College

Development of PVC Reference Materials Containing Hazardous Materials
Matthew Boyce

The Consumer Product Safety Improvement Act (CPSIA) was passed to restrict the levels of hazardous metals in consumer goods. This act restricts total lead mass fraction in children's products to less than 100 parts per million. Due to the broad range of substances incorporated into children's products, new Standard Reference Materials (SRMs) of appropriate matrices are needed for accurate measurements.

Specifically, the Consumer Product Safety Commission (CPSC) has requested the development of a SRM incorporating metals in a poly-vinyl chloride (PVC) matrix. This project seeks to further refine a method of synthesis of these PVC briquettes with lead, cadmium, and titanium incorporated into them. These PVC briquettes can then serve as a new line of PVC SRMs. This project focused on making PVC reference materials which are stable over time and homogeneous. Analysis of these samples was done via X-ray Fluorescence (XRF), with the intention to also use Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS) in future studies.

Worcester Polytechnic Institute

Verification of Zone Fire Models
Brianna Gillespie

Researchers from the Engineering Laboratory at NIST have developed CFAST, the Consolidated Model of Fire and Smoke Transport. CFAST is a two-zone fire modeling program which allows users to predict the environment within a building during a fire, generating data for parameters such as temperature, fire gases, and smoke. Key to the continued use and development of CFAST is confidence that the models it generates are verified and validated. The scope of this research project focused on verification, defined by The American Society for Testing and Materials (ASTM) as “the process of determining that the implementation of a calculation method accurately represents the developer’s conceptual description of the calculation method and the solution to the calculation method”. Simply stated, verification checks that the math within the computer code is correctly implemented.

An initial ‘base case’ model was designed with no use of CFAST features and simple dimensions as a reference model during the verification process. A set of test cases was then developed and CFAST input files were created to demonstrate the range of features that the program can implement. These test cases fell into one of two categories. An ‘Analytical Case’ allowed for a manual solution that tested the use of basic equations in CFAST. A ‘Reference Case’ demonstrated the impact of changing a particular CFAST feature by comparison to the base case model.

Once testing was complete, Matlab was used to graphically present the data. The results of the project were compiled for use in an upcoming NIST Technical Note on verification and validation (V&V) of the model.

Visual Analysis of Fire Spread Rates on Upholstered Furniture Mock-Ups
Mary Long

Fires originating on upholstered furniture represent just 4% of all residential fires in the United States, yet this small percentage accounts for 20% of fire-related deaths and over 25% of property damage. The fabrics and filling materials often used in upholstered furniture can be very flammable, and generate more heat and toxic smoke than fires involving wood or paper products. Studies have been done in the past to support the development of national and state furniture fire safety standards; however the number of lives and property lost remains high. Both open flame tests and smoldering tests have been used to analyze the flammability of furniture materials in the past. Recently, California has proposed a switch to a smolder-only test as a standard for furniture flammability. This proposal stems from concerns about the chemicals used in polyurethane foam that allows current furniture to pass the existing open flame standard test. However, it has been noted in some studies that materials that do well in smoldering tests, like polyester, often do poorly in open flame tests.

The purpose of the work discussed here is to quantify flame spread rates on upholstered furniture through visual analysis. Furniture mock-ups were constructed from four upholstered cushions, and were then ignited using open flames. Eight videos of each assembly and burn were produced including seven different angles and one infrared recording. The mock-ups were assembled from four upholstered cushions arranged in a chair configuration. Twenty different fabric, polyester batting, barrier fabric, and polyurethane foam combinations were tested. The results of the experiment are meant to provide insight about the effectiveness of barrier fabrics and material combinations in open flame tests.

Using graphics and video editing software, flame areas on the back and seat cushions of the mock-ups were isolated as a function of time. The isolated selections were used as inputs to a computational software program written to identify the flame area in terms of pixels. Another program was written determine the actual physical areas corresponding to pixels on the back and seat cushions. The pixel area maps were utilized to convert the pixel areas into physical areas. These calculated areas were then graphed against time as a means to correlate the observed flame spread rates with the material combinations used to construct the cushions.

Yeshiva University

The Reliability of Magnetic Switching in Spintronic Devices
Jonathan Mehlman

Magnetic switching, in which a metal's magnetization switches direction, can be used to store information in a computer. The direction (up or down, for example) of the magnetization can be used to represent a 0 or a 1 and can be easily determined by measuring the resistance across the magnet. Switching between 0 and 1 is accomplished by applying a magnetic field or running a current through the device. The ability to effectively use magnetic switching in computers depends on minimizing the power and time needed to switch a device while maintaining high reliability. Due to thermal effects, switching is probabilistic, which can lead to switching errors. Some memory applications require that there be less than one error in 10^{15} attempts. Therefore, understanding what determines the reliability of magnetic switching is of great interest for engineering usable switching devices. The reliability can be described by the probability that the device fails to switch when intended to. It is important to calculate the probability when errors are rare to determine the limits of power and speed for switching. Studying the evolution of this probability over time as a function of current and temperature provides the necessary information regarding the reliability of switching in the presence of statistical thermal effects. There are no known analytical methods for generally calculating the non-switching probability, requiring the use of numerical approximations. Relying on previous research, we numerically compute the probabilities for a physically symmetric case which greatly simplifies the problem. By identifying key characteristics of these probability distributions, I will present a computationally reasonable way to characterize the reliability of more complex switching mechanisms.

York College of Pennsylvania

Ion Mobility Spectrometry: Characterizing Instrument Response to Drugs as a Function of Desorber Temperature

Jessie Bennett

Ion mobility spectrometry (IMS) has become the most widely used technique for detecting trace narcotics and explosives at checkpoints in prisons and airports nationwide. IMS analyzes particles that have been heated into a vapor by thermal desorption. A radioactive source, Nickel 63, ionizes the neutral vapor as it travels through a weak electric field. Explosives are typically negatively charged while narcotics are typically positively charged. The charged vapor particles will separate based on mass and charge as they reach the detector. The instrument tells the screener whether trace contraband materials were present in the sample.

The goal of this research is to study the instrument's thermal desorption process and its effect on the instrument's response to specific drugs, false alarm rates, and the alarm resolution process. Determining the effect of desorber temperature on instrument sensitivity may identify optimal temperatures for individual narcotics. Cocaine, Meth, THC, and Heroin 0.5 ng to 100 ng) were analyzed at default desorber temperatures on both the Itemiser DX instrument and on the Mobile Trace instrument (235°C and 242°C, respectively). After determining each instrument's characteristic baseline response, the same narcotics were analyzed at varying desorber temperatures (temp range 190°C to 264°C). The Mobile Trace's default temperature may be set too high for Meth yet set too low for THC and Heroin. Due to the narcotics' differing thermochemical properties, some can remain stable at higher temperatures, whereas others may undergo chemical and physical transformations that affect instrument response sensitivity. Results from the DX instrument show that Meth (> 30 ng) begins to decrease in sensitivity around 220°C. More testing will be done to see why this occurs. In conclusion, determining the optimal desorber temperature ranges for individual drugs will allow areas that have a high smuggling rate of specific narcotics to change the default settings in order to target the detection of those specific drugs.

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SURF STUDENTS BY

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UNIVERSITY	STUDENT	TITLE OF TALK	OU
Alabama A & M University	Hinton, Travis	Laboratory Instrument Driver for Residential scale Grid Emulator	PML/ElecEng
Alabama A&M University	Ragland, Tamika	Temporal and Spatial Trends of Perfluorinated Compounds in Ringed Seals *(Phoca Hispida)* from Alaska	MML/NCNR ChemBio
Alfred University	Kutzik, Daniel	All Dressed Up and Somewhere to Go: A SWCNT-Surfactant MD Study	MML/NCNR MatSci
American University	Novy, Melissa	Accelerated Aging of Nuclear Power Plant Cables	EL
Andrews University	Zirkle, Thomas	Improved Signal Generation and Acquisition Methods	PML/ElecEng
Appalachian State University	Aiken, Michael W.	Development of Calibration Standards for Near Infrared Fluorescence Diagnostic Imaging Systems	PML/Physics
Appalachian State University	Hesterberg, Nikolai	Measuring Absorbed Radiation Dose in Water Using Optical Interferometry	PML/Physics
Appalachian State University	Pruett, Zachary	Stellar Photometry: Calibration of Stars	PML/Physics
Arizona State University	Khalil, Osama	Characterization of High Density Plasma Chemical Vapor Deposition Process	CNST
Arizona State University	Lynch, Jenna	A Really Hot Way to Measure Airflow	EL
Arizona State University	Ness, Stuart	Correlations Between Fullerene Miscibility and Organic Photovoltaic Device Performance	MML/NCNR ChemBio
Arizona State University	Ward, Jacob W.	Atomic Spectra of Iron Group Elements: Looking at the Universe Through Atoms	PML/Physics
Augsburg College	Bier, Elianna	Benchmarking the Detection Threshold, Saturation Limit, Linear Dynamic Range, and the Intensity Calibration for a Widefield Fluorescence Microscope Using Fluorescent Glass Reference Materials	MML/NCNR ChemBio
Bates College	Moody, Joanna	Zeta Potential and Particle Size Analysis of Hydrating Cement Solutions	EL
Boise State University	Fritchman, Koyuki	EBSD Strain Measurements of $Si_{1-x}Ge_x$ Thin Films on Si Chips for Reference Material D	MML/NCNR MatSci

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Boise State University	Nelson, Eric B.	Captivating Science: Computational Studies of the Carbon Capture Material HKUST-1	MML/NCNR MatSci
Boise State University	Talley, Kevin R.	Crystal Chemistry and Crystallography of Potential Thermoelectric Perovskites	MML/NCNR MatSci
Brown University	Rosenthal, Anson	A Novel Memory-Efficient Method for Visualizing Large Stitched Images	ITL
Carnegie Mellon University	Buarque de Macedo, Robert	Creating a Testing Infrastructure for Atomistic Simulations of Materials	MML/NCNR MatSci
Carnegie Mellon University	Quintana, Dylan	A Bayesian Approach to Crystal Structure Refinement	MML/NCNR MatSci
Carnegie Mellon University	Spicer, Graham	Fabrication of Nanoporous Aluminum Oxide Films	MML/NCNR ChemBio
Central Washington University	Grist, Richard	Co-W-Al Isothermal Analysis	MML/NCNR MatSci
City College of New York	Bouizy, Zineb	Evaluating Smoldering Ignition Performance of Barrier Fabrics (BF)	EL
City College of New York	Chen, Jing	Hole and Electron Internal Photoemission of MOS Devices	PML/ElecEng
City College of New York	Gauthier, Marilyn	Electrical Transport Measurements of Molecular Layers Using Eutectic Gallium Indium	PML/ElecEng
College of the Holy Cross	Goding, Julian	Analysis of Biodiesel Using Comprehensive Two-Dimensional Gas Chromatography (GCxGC)	MML/NCNR ChemBio
Colorado School of Mines	Glick, Aaron	Modeling Dynamic Elasticity in Dynamic Force Calibration	PML/Physics
Colorado School of Mines	Straley, Tim	Development of a Deep-Level Transient Spectroscopy Data Acquisition Method for Characterization of Photovoltaics	CNST
Cornell University	Bern, Noah A.	Design and Fabrication of a Nano-Scale Cantilever for the Atomic Force Microscope	CNST
Duke University	Liou, Michael	Optimizing 3D Structures for the NIST Chemistry WebBook	MML/NCNR ChemBio
Duke University	Skerritt, Jennifer	Optimizing 3D Structures for the NIST Chemistry WebBook	MML/NCNR ChemBio
Elon University	Zemanick, Amy	Compositional Data Analysis of a Cement Clinker	ITL
Florida A & M University	Kelley, Ronisha	Digital Multimeter Calibrations	PML/ElecEng

UNIVERSITY	STUDENT	TITLE OF TALK	OU
George Washington University	Fusco, Emily	From the Redwood Forest to the Gulf Stream Waters: Creating a Database of Spectral Solar Data Via Locations Spanning the U.S.	EL
George Washington University	Soberman, Danielle	A Study of Polymer Interactions at the Membrane-Solution Interface for Single Molecule DNA Sequencing Applications	PML/ElecEng
Georgetown University	Burton, George	Synthesis and Microscopic Characterization of Anisotropic Colloids and Induced Depletion Interactions	MML/NCNR ChemBio
Georgetown University	Dougherty, Timothy P.	Solving Our Carbon Dioxide Problem: CO_2 Binding in Metal-Organic Frameworks	MML/NCNR MatSci
Georgia Institute of Technology	Carlson, Max	Conceptual Design of a High-Power, Low-Enriched Uranium (LEU) Research Reactor	MML/NCNR MatSci
Georgia Institute of Technology	Clawson, Aidan Z.	Performance Characterization of Precision Positioning Systems	EL
Gustavus Adolphus College	Seberson, Troy	Characterization and Optimization of Neutron Polarization and Magnetic Field for a Neutron Electric Dipole Moment Experiment	PML/Physics
Hamilton College	Wilson, Brandon	Towards Microgram Mass Standards for Small Force Metrology	PML/Physics
Harvey Mudd College	Baeder, Michael A.	Generalizations of Generating Functions for Hypergeometric Orthogonal Polynomials	ITL
Hood College	Paxton, Alex	A Preliminary Testbed Architecture Design for the Sustainable Manufacturing Testbed	EL
Hood College	Staples, Robert	Software Entropy Sources for Cryptographic Applications	ITL
Indiana University	Lamadokou, Kwami	Friction Effect on Displacement of a Cantilever Beam-Based Instrument During Polymerization Shrinkage	MML/NCNR MatSci
Interamerican University of Bayamón Puerto Rico	De Jesús, Ramón L.	Measuring Software Performance on Mobile Devices	ITL
Inter-American University of Puerto Rico	Morales-Otero, Michael	Density of States Characterization in Single Crystals of Rubrene	PML/ElecEng
James Madison University	Leaman, Eric	Characterization of NIST-4 Components and Materials	PML/ElecEng

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Johns Hopkins University	Sampson, Isaiah	Structural Robustness of Reinforced Concrete Frames	EL
Johns Hopkins University	Skerritt, Elizabeth	Fabry-Perot Displacement Interferometry in Air	PML/Physics
Johns Hopkins University	Wheatley, Rebekah	Fourier and Gegenbauer Expansions of a fundamental solution of Laplace's Equation on a Hypersphere	ITL
Juniata College	McGrew, William F.	Rydberg Rubidium Atoms for Charge Exchange in a Penning Trap	PML/Physics
Kansas State University	Blankenau, Brian	Evaluation of a Diamagnetic Levitation Apparatus for Determining AFM Force Calibration Factors and Spring Constants	CNST
Lehigh University	Stritch, Kyle	Microanalysis of Various Materials Deposited by Atomic Layer Deposition	MML/NCNR MatSci
LeMoyne College	Emma D'Ambro	Dynamical Structure Measurements of Biotherapeutics with Hydrogen/Deuterium Exchange Mass Spectrometry	MML/NCNR ChemBio
LeMoyne College	Marshall, Erin	Boise-Einstein Condensation of Photons	PML/Physics
Lock Haven University	Leber, Kyle	The Tale of Two Models	ITL
Louisiana State University and A&M College	Brignac, Chase	Optimal Photon Down-Conversion Through Thermal Control of Nonlinear Crystals	PML/Physics
Massachusetts Institute of Technology	Ok, Meryem Tyrrasch	Investigation of the Potential Genotoxicity of Acid-Modified NanoTitania	MML/NCNR ChemBio
Miami Dade College	Moser, Markus	How to Calibrate a Digital DC-MM-Calibrator Effectively	PML/ElecEng
Montgomery College	Al Ammary, Rehab	Identifying Critical Links in a Network	ITL
Montgomery College	Al Ammary, Sarab	Error Analysis on OpenHaRT13 Evaluation	ITL
Montgomery College	Movius, Ian	Development of an Apparatus to Measure the Optical Properties of Black Carbon Ice Nuclei	MML/NCNR ChemBio
Montgomery College	Nguyen, Trinh	New and Rapid Methods to Measure Viability of Bacterial Biofilms	MML/NCNR ChemBio
Montgomery College	Safi, Taqiyyah	Integration of Adaptive Control in Cyber Physical Systems for Enhanced System Performance	EL

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Mount St. Mary's University	Dockery, Lance	Determination of Aggregate Size Dependence Effect on Soot Particle Packing in a Macroscale Experiment	MML/NCNR ChemBio
Muhlenberg College	Rommal, Andrea	Investigation of Trevisan Extraction Theory and Framework	ITL
North Carolina State University	Frame, Dillon	Shielding Designs for a Short-Baseline Neutrino Detector: A Monte Carlo Approach	PML/Physics
North Carolina State University	Waller, Jackson	Molecular Self-Assembly in Water-Alcohol Solutions	MML/NCNR MatSci
Northwestern University	Wolff, Sarah	Sustainable Manufacturing Standards Ontology	EL
Oberlin College	Fein, Mira	Redefining Acceptable White Light for General Lighting	PML/Physics
Oberlin College	Sharpe, Samuel	Environmental and Economic Sustainability of Residential Buildings	EL
Ohio Northern University	Skobrak, Kathryn	Machine Tool Performance Under Loaded Conditions	EL
Oklahoma State University	Seader, John	Solution Chemistry and Kinetics of High Volume Fly Ash Binders	EL
Polytechnic University of Puerto Rico	Ortiz, Manuel	WiFi Indoor Localization	ITL
Princeton University	Breen, Catherine	Automating Image Edge Detection with Accuracy comparable to Manual Reference and Correlating Oct4 GFP Gene Reporter Expression with Antibody Label for Oct4 in Stem Cell Colonies	ITL
Purdue University	Epling, John	Standard Reference Mortar Development	EL
Reed College	Khader, Isaac	Reactor Data at Your Desk	MML/NCNR MatSci
Rensselaer Polytechnic Institute	Novotny, Whitney	Thermal Processing Impacts on Slow Growth Resistance of High density Polyethylene	EL
Rochester Institute of Technology	Weinstein, Perri	Evaluation of Thiolacetates and Disulfides as Lipidic Anchors in Tethered Bilayer Membranes (tBLMs)	MML/NCNR ChemBio
Rowan University	Kassner, Christopher	Measurement of Magnetic Anisotropy in in Magnetic Nanoparticles	MML/NCNR MatSci

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Rowan University	Smith, Troy	Improved Data Comparison Schemes for Inter-Laboratory Studies on High-Pressure Gas Sorption Data	MML/NCNR MatSci
Rutgers University	Sytwu, Katherine	Optical Ferromagnetic Resonance Measurement Using the Kerr Effect	CNST
Savannah State University	Brooks, Sterling	Measurement Science for Concrete Surface Electrical Resistivity Test Methods	EL
Savannah State University	Simpore, Leticia	Automation of Performance Plan Generation	EL
Smith College	Stoudt, Sara	Measuring Optical Apertures for Solar Irradiance Monitoring	ITL
Smith College	Udwin, Dana	Face Recognition Performance in Point-and-Shoot Videos	ITL
Southern University A & M College	Jones-Butts, Shannon	Chemical Structure – Performance Relationships of Molecular Layer by Layer Water Desalination Membranes	MML/NCNR MatSci
State University of New York Albany	Briggs, Michael C.	Photoresist Surface Modification for Photolithography	CNST
State University of New York Albany	Brisbois, Chase	Probe-Assisted Doping and the World's Smallest QR Code	PML/ElecEng
State University of New York Binghamton	Gladstone, Jessica	Optical Measurements of Porosity in Additive Manufactured Metallic Parts	EL
State University of New York Binghamton	O'Brien, Edward	Designing a 100TΩ Standard Resistor	PML/ElecEng
State University of New York Binghamton	Watrobski, Paul	High-Speed RF Spectrum Analysis on a Software-Defined Radio	ITL
State University of New York Binghamton	Wong, Andrew	Massively Parallel Long Term Reliability System	PML/ElecEng
State University of New York Binghamton	Wong, Daniel	Laboratory Instrument Driver for Home Area Energy Network	PML/ElecEng
State University of New York Stony Brook	Ging, James	Fuzzy Fiber Fillers: Understanding the Metrology and Aquatic Durability of the Next Generation of Polymeric Nanocomposites	EL
Swarthmore College	Cosentino, Justin	Extrinsic Lidar Calibration for Use with Mobile Robotics	EL
Swarthmore College	Nahmias, David	Design, Construct and Test a Computer Controlled Mannequin Mover for Automated Guide Vehicle A(AGV) Obstacle Avoidance Measurements	EL

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Swarthmore College	Weck, Peter	Detecting Nanoscale Three-Dimensional Shape Variations Using an Optical Microscope	PML/Physics
Texas A & M University Corpus Christi	Hernandez, Christopher	Utilizing Infrared Spectroscopy for the Investigation of Organic Photovoltaic Formation	MML/NCNR ChemBio
Towson University	Jay, Emily	Security of WS-Biometric Devices (WS-BD)	ITL
University of California Berkeley	Hwang, Kenneth	A Review won Additive Manufacturing Processes	EL
University of California San Diego	Krayer, Lisa	Etch Damage in Magnetic Thin Film Head Materials	MML/NCNR MatSci
University of Delaware	Fleischman, Marianna	An Investigation of the Stabilizing Effects of Surfactants on Bio-Therapeutics	MML/NCNR MatSci
University of Evansville	Bashor, Ian	Performance Testing for Android Devices for Tactical Military Use	EL
University of Florida	Carter, Jared	Synthesis and Crystal Structure of $Na_{(1-y)}Li_yNb_{(1-x)}Ta_xO_3$	MML/NCNR MatSci
University of Florida	Correa, Luis Felipe	Indentation Metrology for Nanomechanical Properties	MML/NCNR MatSci
University of Florida	Fong, Grant	Remote Controlled Vacuum Instrumentation of the Cold Neutron Source	MML/NCNR MatSci
University of Illinois Urbana-Champaign	Shirley, Wilbur	Half-Quantized Vortex Molecules in Quasi-Two-Dimensional Rotating Binary Superferrofluids	PML/Physics
University of Illinois Urbana-Champaign	Tretternero, Philip	Measuring the Defect Density of Carbon Nanotubes	CNST
University of Illinois Urbana-Champaign	Willi, Joseph	Behavior of Fire Fighter Polycarbonate Personal Protective Equipment in Extreme Heat Conditions	EL
University of Kentucky	Hackett, Benjamin	Improving the 3-D Metrological Capabilities of the SEM	PML/ElecEng
University of Maryland Baltimore County	Austin, Natalie	Understanding Intracellular Biomineralization: Exploring the Role of pH and Supersaturation on the Composition of Amorphous Calcium Phosphate	MML/NCNR MatSci
University of Maryland Baltimore County	Bishoff, Michael	Heterogeneous Mapping Platform for Model-Based System Engineering	EL
University of Maryland Baltimore County	Dhanasekaran, Vignesh	Monitoring Magnetic Levitation Through Interferometry	PML/ElecEng

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University of Maryland Baltimore County	Drew, Celia	Mobility Management for Heterogeneous Networks	ITL
University of Maryland Baltimore County	Kumar, Neha	Growth Factor Deliverable Smart Nanofiber Scaffolds for Tissue Engineering Applications	MML/NCNR MatSci
University of Maryland Baltimore County	Luu, Peter	Effect of Reduced Beam Divergence on NIST Ozone Standard Reference Photometer Measurements	MML/NCNR ChemBio
University of Maryland Baltimore County	Murali, Danya	Creating Profiling Tools to Analyze and Optimize FiPy	MML/NCNR MatSci
University of Maryland Baltimore County	Smith, Nathan	Optimization of Modeling of MIS Devices for Solar Energy Conversion	MML/NCNR MatSci
University of Maryland College Park	Ambalavanar, Guru Ram	Resource Public Key Infrastructure (RPKI) Deployment Strategies and Its Impact on Today's Backbone Routing	ITL
University of Maryland College Park	An, Wasson	Computer Assisted Translator for SPAF	EL
University of Maryland College Park	Badger, Andrew	Cryptography in Constrained Environments	ITL
University of Maryland College Park	Bajcsy, Andrea	From Web Graphics to 3D Haptics: Depicting Web Images for the Blind and Visually Impaired	ITL
University of Maryland College Park	Boger, Shir	Characterization of Microfabricated Particles and Protein Aggregates Using a Custom Microfluidic Coulter Device	MML/NCNR ChemBio
University of Maryland College Park	Chuang, Kevin	Thinking Green: Sustainable Energy Modeling for Arc Welding Processes	EL
University of Maryland College Park	Clagg, Justin	Creating an Efficient Program to Simulate Dynamics of One-Dimensional Quantum Many-Body Systems	PML/Physics
University of Maryland College Park	Connolly Kathryn	Durability of PET in Photovoltaic Applications	EL
University of Maryland College Park	Elahi, Syed	Database Automation by Solving Puzzles!!!	EL
University of Maryland College Park	Elkin, Rena	The Importance of User-Friendly Interfaces for Public Resources	EL
University of Maryland College Park	Etkins, Ryan	Improving Sustainability Analysis of Unit Manufacturing Processes	EL
University of Maryland College Park	Faenza, Nicholas	Multi-Substrate Flammability Reduction Using a Layer-by-Layer Assembly with Natural Materials	EL

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University of Maryland College Park	Gan, Cynthia	Content-Based Image Comparison	ITL
University of Maryland College Park	Golshany, Fardad	Electrical Modeling of the Change in Resistance in Through-Silicon Via Daisy Chain Subjected to Thermal Cycling	PML/ElecEng
University of Maryland College Park	Hafner, Katie	Optimizing 3D Structures for the NIST Chemistry WebBook	MML/NCNR ChemBio
University of Maryland College Park	Hamins-Puertolas, Adrian	Estimating the Cost of Inadequate Interoperability for Manufacturing Processes	EL
University of Maryland College Park	Hitz, Emily	COMSOL Simulation of Multi-Level Interconnects for Advanced Integrated Circuit Design	PML/ElecEng
University of Maryland College Park	Huang, Eric	Microelectromechanical Triaxial Accelerometer Testing	PML/ElecEng
University of Maryland College Park	Jamgochian, Arec	Exploring the Sapphire Whispering Gallery Thermometer	PML/Physics
University of Maryland College Park	Jones, Benjamin	Graphitic Carbon Thin Films for Neutron Reflectometry Investigations of Rechargeable Batteries and Fuel Cells	MML/NCNR MatSci
University of Maryland College Park	Keller, Kevin	Stampeding Over Cement: Simulating Chemical Kinetics in Parallel with HydratiCA	ITL
University of Maryland College Park	Khalid, Mian	Flexible Conducting Polymer Actuators for Cell Stimulus Applications	PML/ElecEng
University of Maryland College Park	Kim, Byung	Metrology of Force-Based Control for Robotic Assembly	EL
University of Maryland College Park	Kravitz, Nadav	Raman Analysis of Carbon Nanostructures	PML/ElecEng
University of Maryland College Park	Krummel, Gregory	Hand-Arm Coordination: Integration and Control of Dexterous Robots	EL
University of Maryland College Park	Kundu, Anita	The Effect of the Hydration Layer on the Small Angle Scattering Data of Proteins	MML/NCNR MatSci
University of Maryland College Park	McPartland, Kari	Membranes for Clean Water: Developing a Cure for Chlorine Degradation	MML/NCNR MatSci
University of Maryland College Park	Murty, Eshwari	Electrochemical Deposition of Pt_3Ni Ultrathin Film Catalysts for PEM Fuel Cells	MML/NCNR MatSci
University of Maryland College Park	Nouketcha, Franklin	Measuring and Modeling Parasitic Resistances in CMOS Transistors	PML/ElecEng

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University of Maryland College Park	Oeste, Tom	The Impact of Robot-Human Collaboration	EL
University of Maryland College Park	Omori, Hidemi	Improving Emergency Evacuation Effectiveness	EL
University of Maryland College Park	Onyenemezu, Charles	Engineering Polymer Fiber 3D Composite Scaffolds for Enhanced Periodontal Tissue Regeneration	MML/NCNR MatSci
University of Maryland College Park	Ruppel, Emily	Measuring the Power Supply of the Future	PML/ElecEng
University of Maryland College Park	Shyu, DoRonne	In Situ Characterization of Polymer Adsorption Properties Using Quartz Crystal Microbalance	MML/NCNR MatSci
University of Maryland College Park	Siegel, Jacob	Virtual Calibration: Using an iPhone to Calibrate Multiple Microscopes	ITL
University of Maryland College Park	Sineriz, George	Controlled Optical Levitation of Small Particles	PML/ElecEng
University of Maryland College Park	Tolstaya, Ekaterina	Measurements of a Copper Polypeptide Solar Fuels Catalyst	CNST
University of Maryland College Park	Tselenchuk, Dimitri	Development of Silver Nanocomposite Model Systems to Test for Environmentally Induced Nanoparticle Release	MML/NCNR ChemBio
University of Maryland College Park	Villarrubia, Mark	Evaluating a Machine Learning Algorithm for Spam Detection Through Standardizing Spam Characterization	ITL
University of Maryland College Park	Walsh, Benjamin	Design and Construction of a Differential Current Amplifier for Capacitance Measurement with an Atomic Force Microscope Probe	PML/ElecEng
University of Maryland College Park	Wang, Grace	Improving Quantitative Immunostaining Measurements by Atomic Force	MML/NCNR MatSci
University of Maryland College Park	Wiess, Emily	Analysis of Stairwell Evacuation	EL
University of Maryland College Park	Zubajlo, Rebecca	Utilizing Microfluidic Platforms to Develop Microbial Pathogen Separation Techniques	MML/NCNR ChemBio
University of Missouri Kansas City	Regina, Jason	How to Blow a House Down: Confessions of the Big Bad Wolf	EL
University of Puerto Rico	Conklin, Steven	Neutron Diffraction Study of Pressure-Dependent Magnetism in Molecule-Based Magnets	MML/NCNR MatSci

UNIVERSITY	STUDENT	TITLE OF TALK	OU
University of Puerto Rico	Santillan, Jaime	Collection of Standard Reference Data for Gas Adsorption via Molecular Simulation and Literature Meta-Analysis	MML/NCNR MatSci
University of Puerto Rico Mayaguez	Molina Serrano, Kevin	Manufacturing Sensor Knowledge Representation	EL
University of South Alabama	Hill, Haley	Sustainable Thinking in the Design Environment	EL
University of South Florida	Byrnes-Blanco, Laura	SI Traceable Calibration of Thermal Cantilever Vibrations in a LDV	MML/NCNR MatSci
University of Texas Austin	Jaffe, Gabriel	Automating Tunnel Junction Device Fabrication	PML/Physics
University of Texas Austin	O'Kelly, Devin	Neutron Vision	PML/Physics
University of Texas Dallas	Borner, Katherine	Investigation of Stability of Silica Particles in Lutidine/Water Solvent	CNST
University of the District of Columbia	Jinfessa, Jote	High-Throughput Photovoltaic Efficiency Testing Rig	MML/NCNR MatSci
University of Virginia	Harinder, Arvind	Requirements Analyses to Support a Material Information Model for Sustainability	EL
University of Virginia	Yang, Alexander	Developing Ontologies Through a Root-Based Vocabulary in a Semantics Database	MML/CNR ChemBio
University of Washington	Kearns, Rachel	An Optical Force-to-Frequency Transducer	PML/Physics
University of Wisconsin Platteville	McIlree, Joseph	A Case Study of a Turning Machine to Validate Sustainable Process Analytic Formalism	EL
Vanderbilt University	Russell, Theodore	Energy Optimization of Welding Operations	EL
Virginia Polytechnic Institute & State University	Bass, Lindsey	Measurement Deviations of Additively-Manufactured Parts from Their Theoretical Models	EL
Virginia Polytechnic Institute and State University	Webster, Kelly	CFD Simulation of Flow Around Bluff Body Objects	EL
Virginia State University	Batson, Bruce D.	Inheritance in Attribute Control Policy	ITL
Virginia State University	Kakal, Taher	3D Topography Analysis of 10 Consecutively Manufactured Drift Punches	PML/ElecEng
Virginia State University	Williams, Janelle	Digital Repository of Mathematical Formulae	ITL
Virginia State University	Wood, Imani	Functionalized Gold Nanoparticles That Resist Protein Adsorption	MML/NCNR ChemBio

UNIVERSITY	STUDENT	TITLE OF TALK	OU
Virginia Wesleyan College	Boyce, Matthew	Development of PVC Reference Materials Containing Hazardous Materials	MML/NCNR ChemBio
Worcester Polytechnic Institute	Gillespie, Brianna	Verification of Zone Fire Models	EL
Worcester Polytechnic Institute	Long, Mary	Visual Analysis of Fire Spread Rates on Upholstered Furniture Mock-Ups	EL
Yeshiva University	Mehlman, Jonathan	The Reliability of Magnetic Switching in Spintronic Devices	CNST
York College of Pennsylvania	Bennett, Jessie	Ion Mobility Spectrometry: Characterizing Instrument Response to Drugs as a Function of Desorber Temperature	MML/NCNR ChemBio

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