Greetings!

On behalf of the Director's Office, it is my pleasure to welcome you to 2016 SURF Colloquium at the NIST Gaithersburg campus.

Founded by scientist in the Physics Laboratory (PL) with a passion for stem outreach, the SURF Program has grown immensely since its establishment in 1993. The first cohort of the SURF Program consisted of 20 participants from 8 universities primarily conducting hands-on research in the physics lab. Representing all STEM disciplines, this summer's cohort of the SURF Program includes 188 participants from 100 universities engaging in research projects in all 7 laboratories at the Gaithersburg campus. It's expected that the program will continue to grow in the future.

During your attendance at the SURF Colloquium, I encourage you to interact with the SURF participants. Aside from asking questions during the sessions, I recommend networking with presenters in between sessions and/or lunch. The colloquium is the perfect venue to exchange findings and new ideas from the most recent and rigorous research in all STEM fields.

Furthermore, I suggest chatting with NIST staff and scientist at the colloquium. Don't be afraid to ask questions about the on-going research in a specific NIST laboratory. Most staff and scientist love to talk about their role or research at NIST.

Moreover, I invite you to share your experience at the SURF Colloquium on the National Institute of Standards and Technology (NIST) Facebook page using the hashtag, #2016SURFColloquium.

Lastly, I could not conclude this letter without mentioning the individuals which make the SURF Program at NIST possible. Thank you to the OU SURF Directors, the SURF mentors, and all the staff at NIST who play an integral role in making the SURF participants experience valuable. Your hard work and dedication to the program is greatly appreciated.

Again, welcome to the conference. I'm glad that you are here and I look forward to your participation in the SURF Colloquium.

Warm regards,

Brandi K. Toliver

Brandi Toliver, PhD
Managing SURF Program Director (NIST-wide)

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NIST SURF Program Staff by Organizational Unit (OU)

Organizational Unit (OU)	Name
Director's Office	Brandi Toliver, Managing SURF Program Director
Director's Office	Kara Arnold
Center for Nanoscale Science and Technology	John Unguris
Center for Nanoscale Science and Technology	Kartik Srinivasan
Engineering Lab	Lisa Jean Fronczek
Information Technology Lab	Howard Cohl
Information Technology Lab	Elizabeth Lennon
Information Technology Lab	Derek Juba
Information Technology Lab	Michaela Iorga
Communications Technology Lab	David Griffith
Material Measurement Lab	Rebecca Zangmeister
NIST Center for Neutron Research	Julie Borchers
NIST Center for Neutron Research	Joseph Dura
Physical Measurement Lab-Electrical Eng	Joseph Kopanski
Physical Measurement Lab-Electrical Eng	Richard Steiner
Physical Measurement Lab-Electrical Eng	Darwin Reyes-Hernandez
Physical Measurement Lab-Physics Lab	Cameron Miller
Physical Measurement Lab-Physics Lab	Uwe Arp
Physical Measurement Lab-Physics Lab	Maritoni Litorja
Physical Measurement Lab	Anita Sweigert
Standards Coordination Office	Nathalie Rioux

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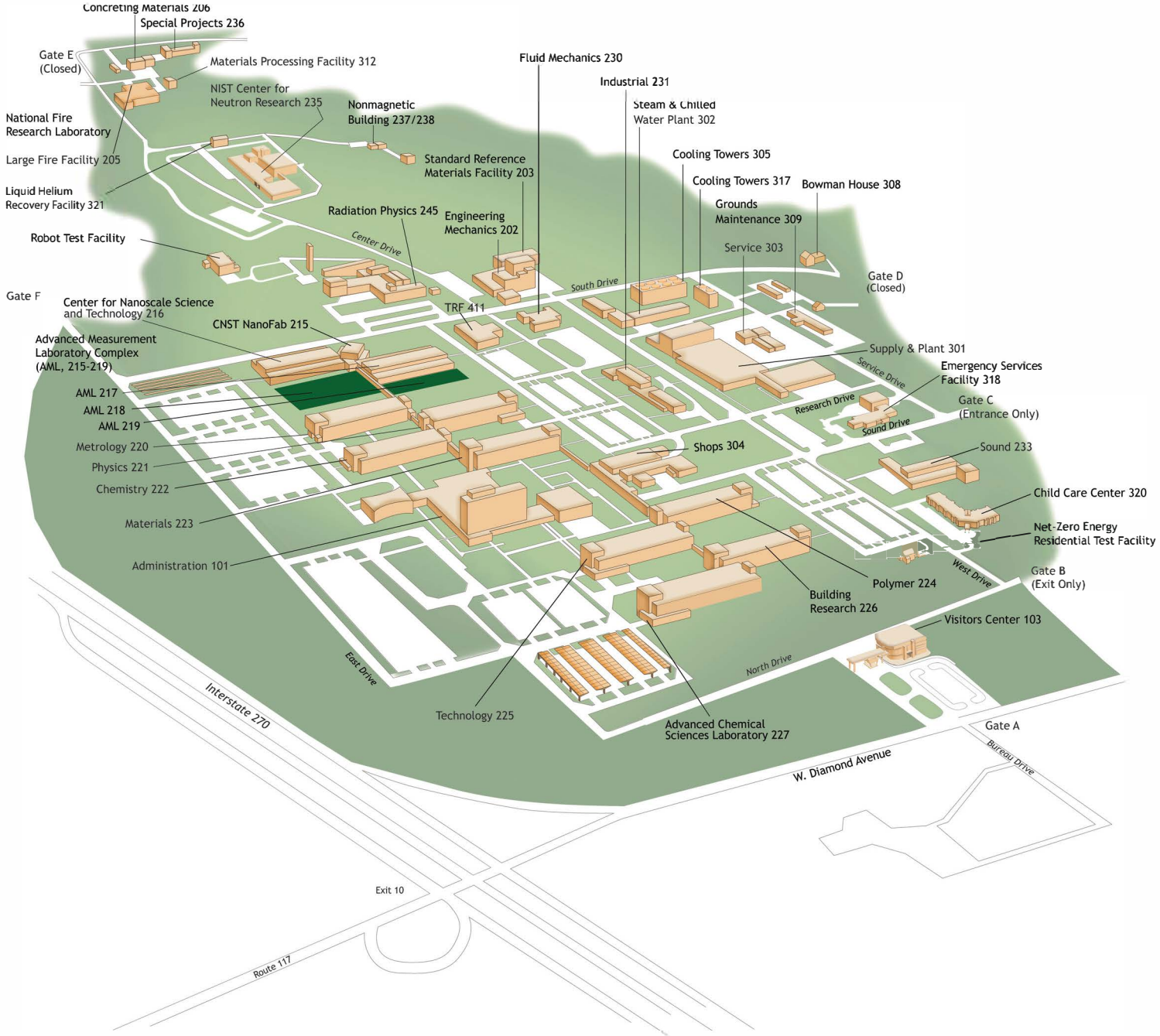
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SURF Colloquium: Tuesday, August 2, 2016

Plenary Session: Green Auditorium, Administration Building (101)

Time	Agenda
9:00A	**Welcome** *Dr. Kent Rochford*, NIST Associate Director for Laboratory Programs
	Session Moderator *Dr. Brandi Toliver,* Managing SURF Program Director
9:15A	**CNST** *Kimberly (Kimi) Bourland*, Exploring Li-ion Battery Materials with Focused Ion Beams
9:45A	**EL** *Tony Zhang,* Onboard Location Tracking for Collaborative Robot Applications
10:15A	**ITL/CTL** *Sean McHugh,* A Meta-Analysis on Super-Recognizers: Experts in Facial Recognition
10:45A	**MML** *Keith White,* Engineering of Nano-Carbon Graphene Based Devices & the Effect of Atmospheric Dopants on Graphene's Electronic Properties
11:15A	**NCNR** *Abdullah Weiss,* Compton Suppressed Gamma Spectroscopy of Spent Fuel from NBSR
11:45A	**PML** *Jacob Ward***,** Energy Level Optimization of Quadruply Ionized Nickel (Ni V)
12:15P	**Special Programs** *Anna Gilpin,* What is the Meaning of Life?: Terminology and Measurement Assurance for Biotechnology Standards
12:45P	**Lunch -** Dining Rooms A & B: Meet the SURF directors and external visitors

SURF Colloquium: Tuesday, August 2, 2016

Parallel Sessions Agenda: MML/NCNR-MatSci and ITL/CTL

	MML/NCNR_MatSci	**ITL/CTL**
	Location: Lecture Room B	**Location: Lecture Room D**
Time	Moderator: Julie Bitter	Moderator
2:20P	*Samuel Underwood*: Silver Nanoparticle-embedded Textiles: Preparing and Characterizing a Model System	*James Rogers*: Injection Preservation: Testing Code with Injected Vulnerabilities for Expected Results
2:40P	*Sydney Brooks*: Fiber Trace Evidence: Quantification of Sample Bleaching During UV-vis Microspectrophotometry	*Bruce James*: Out of Time: Abstracting Temporal Constraints from Time-Based Data in Non-relational Databases
3:00P	*Erica Lee*: Durability of Carbon Nanotube Reinforced Alumina Fiber - Epoxy Composites	*Joie Murphy*: Implementing distributed interfaces: tools from natural language and mathematics
3:20P	*Sarah Smith*: Potential Age Dating of Fingerprints using Time-of-Flight Secondary Ion Mass Spectrometry: Looking at the Diffusion of Fatty Acids on Model Surfaces that Mimic Real World Surfaces	*Ryan Smith*: Accelerating k-D Trees for Nearest Neighbor Search in Walk-on-Spheres
3:40P	*Heetae Jeon*: The Unique Functions of Urethane dimethacrylate in Photo-copolymerization with an Ether-based Divinylbenzyl Monomer	*Kyle Sutton*: Inside a Meteorite: Volume Estimation from the Segmentation of Cross-Sectional Images
4:00P	*Lauren Singer*: Engineering a Low Cost, Open Source Electrospinning System for Nanofiber Production	*Sean Strange*: Developing and Testing the Spectrum Access System: Path to Effective Spectrum Sharing
4:20P	*Andrew Gayle*: Nano-Scale Strain Mapping in Three Dimensions	*Steven Smith*: Calculation of Exclusion Zones for Radar Protection in the 3.5 GHz Spectrum Band
4:40P	*Andres Correa Hernandez*: Density Functional Theory Studies of Nanoporous Materials	*David Indictor*: Machine Learning for Spectrum Prediction

SURF Colloquium: Tuesday, August 2, 2016 (Afternoon)

Parallel Sessions Agenda: ITL/CTL

	MML/NCNR-ChemBio
	Location: Lecture Room A
Time	Moderator: Rebecca Zangmeister, MML/NCNR SURF Director
2:20P	*Cristopher Hernandez Macias*: Observing Trypsin-Catalyzed Transpeptidation Products Using UHPLC-MS
2:40P	*Emily Jin*: Engineering Biology, Using Bioinformatics to Predict N-Linked Glycosylation Sites in Proteins
3:00P	*Cayla Collet*t: Protein Aggregation: Characterizing Particles Formed in Therapeutic Protein Drugs
3:20P	*Aaron Bezio*: Development of the Next Generation of Hydrogen/Deuterium Exchange Mass Spectrometry Apparatus
3:40P	*Natalie McDonald*: Characterization of protein aggregation using Asymmetric Flow Field Flow Fractionation (AF4) and Multi-Angle Light Scattering (MALS)
4:00P	*Connor Galvin*: Exploring a Novel pH-based Strategy for Protein Crystallization
4:20P	*Jessica Young*: Study of Interaction of Peptides with Tethered Bilayer Phospholipid Membranes
4:40P	*Emmie Knobloch*: Assessing Standard Assays for Cytotoxicity of Dental Materials
5:00P	**END**

SURF Colloquium: Tuesday, August 2, 2016 (Afternoon)

Parallel Sessions Agenda: EL and PML-Physics Lab

	EL	PML-Physics Lab
	Location: Heritage Room	**Location: Portrait Room**
Time	Moderator:	Moderator: C. Cameron Miller, PML SURF Director
2:20P	*Philip Hoddinott*: Design and Construction of Intelligent Building Agent Laboratory	*Hannah Hastings*: Not All AC Power Supplies Are Equal, According to an LED Source
2:40P	*Robert Leader*: Tools for the Ongoing Commissioning of Buildings	*Samuel Brown:* Standardizing Firefly Luminescence
3:00P	*Rachel McIntyre*: Temperature Dependent Measurements of Photovoltaic Solar Cells	*Daniel Paseltiner:* Development of a Digital Holographic Microscope for Imaging Bose-Einstein Condensates
3:20P	*Matthew Parsons*: Quantitive Analysis of Cement Paste Performance via Oscillatory Rheology	*Keeley Townley-Smith:* Line identification and level analysis of Ti II in the ultraviolet region
3:40P	*Daniel Kamieniecki*: 3D Printing Cement: Characterization of Printable Cement Pastes	*Joshua Hanson:* Capturing Highly Charged Ions in a Radio-Frequency Paul Trap
4:00P	*Behailu Kifle*: Phase Analysis of Portland Cement Clinker by Scanning Electron Microscopy and X-Ray Powder Diffraction	*Joshua Graybill:* Excimer-based Neutron Detection using Far Ultraviolet Noble Gas Emission
4:20P	*Stephen Caren*: Artificial Sunny Days: Impact of Temperature on Polyethylene Photodegradation Under Accelerated Weathering	
4:40P	*Samantha Weaver*: Impacts of Temperature, Relative Humidity, and UV Source on EVA Degradation in Accelerated Weathering Tests	

SURF Colloquium: Wednesday, August 3, 2016 (Morning)

Parallel Sessions Agenda: MML/NCNR-MatSci and ITL/CTL

	MML/NCNR-MatSci	ITL/CTL
	Location: Lecture Room B	**Location: Lecture Room D**
Time	Moderator:	Moderator:
9:00A	*Timothy Barret*: Uncertainty of the Impulse Excitation Technique	*Eric Dougherty*: Virtual Reality on the World Wide Web
9:20A	*Anushka Dasgupta*: Evaluating the Accuracy of Phase Field Codes Using Community-Developed Standard Benchmark Problems	*Vinay Sriram*: Sampling Techniques to achieve Color Fidelity and Anti-aliasing in the Conversion of Cubic Maps to Spherical Maps for Virtual Environments
9:40A	*Aline Elquist*: New Models for Electrochemical Systems	*Dan Dunkers*: Using the CIE-LAB color space to improve the analysis of tests across system differences for the CAVE (Computer Assisted Virtual Environment)
10:00A	*Michael Locke*: Characterizing Material Behavior Via High-Rate Mechanical Testing Using a Split Hopkinson Pressure (Kolsky) Bar and Pulse Heating System	*Justin Mayer*: Investigating the mechanics of failure through visualization
10:20A	*Austin Schuberth*: Finite Element Modeling	*Derrick Addo*: Synchronizing Video Playback on a Tiled Display Wall
10:40A	BREAK	BREAK
	Moderator	Moderator
11:00A	*James Boligitz*: Investigation of phase equilibria in binary Co-W surrounding the μ-phase via mechanical alloying	
11:20A	*Sarah Hood*: Domain Structures and Dynamics of Polar Ordering in Pb(〖Sc〗_(1/2) 〖Nb〗_(1/2))O3 with Pb-O Divacancies	
11:40A	*Norman Luu*: Property Calculations Within the Interatomic Potentials Repository Framework	
12:00N	*Andrey Moskalenko*: Developing the Cloud of Reproducible Records (CoRR) and evaluating its performance compared to existing tools	
12:20P	*Karina Stetsyuk*: Adding automated uncertainty estimates to temperature- and pressure-dependent property calculations of iron from molecular dynamics	
12:40P	**LUNCH**	**LUNCH**

SURF Colloquium: Wednesday, August 3, 2016 (Morning)

Parallel Sessions Agenda: EL and PML-Physics Lab

	EL	PML-Physics Lab
	Location: Heritage Room	**Location: Portrait Room**
Time	Moderator:	Moderator: Uwe Arp, PML SURF Director
9:00A	*Justin Goh*: Simulation Assisted Robot Hand and Arm Programming for Planning and Simplifying User Experience	*Peter Walecki*: Radiation Dose Metrology through Water Calorimetry
9:20A	*Omar Aboul-Enein*: Augmented Reality Marker Tracking for Multi-Robot Registration	*Joshua Edgerton*: Quantification of PET Imaging Using NIST-calibrated Radionuclide Sources
9:40A	*Patrick Seiler*: Assessing the Impact of Cybersecurity on Networked Control Systems	*Ben Riley*: An Evaluation of a Dual-Energy Method for CT Imaging
10:00A	*Theodore Johnson*: Control System Implementation for Motorized Dynamic Bending and Calibration Machine	*Robert Valdillez*: Measuring the Neutron Spectrum of 250Cf with a Time of Flight Measurement
10:20A	*Christina Krueger*: Seeing between the Lines: Layerwise Imaging for Metal Additive Manufacturing	*Benjamin Schafer*: Neutron Polarization Measurement on the NG-C Beamline for aCORN
10:40A	**BREAK**	**BREAK**
	Moderator:	Moderator: Uwe Arp, PML SURF Director
11:00A	*Shawn White*: Dynamic and Mechanical Properties of Metal Powder	*Samuel Brandt*: Measurement of Schwinger Scattering in Silicon
11:20A	*Adam Springer*: Dynamic Characteristics of the Recoater Arm used in the Direct Metal Laser Sintering Process instead of Dynamic Characteristics of the Recoater Arm used in the Powder Bed Fusion Process	*Lindsey Barner*: Machining of Fluidic Structures with Helium Ions
11:40A	*Alexander Stoddard*: Squareness - Numerical Errors in The Utilization of Machine Tools for Engineering Processes	*Samuel McClung*: Unusual Phenomena in Convective and Sonic Gas Flows
12:00N	*Matlock Mennu*: Sensor-Based Diagnostics of CNC Linear Axes	*Maxwell Lindsay*: Controlled carbon nanotube functionalization for assessing origin of Raman D-band components
12:20P	*Thomas Winnard*: CNC Linear Axis Diagnostics via Sensors	
12:40P	**LUNCH**	**LUNCH**

SURF Colloquium: Wednesday, August 3, 2016 (Afternoon)

Parallel Sessions Agenda: MML/NCNR-MatSci and ITL/CTL

	MML/NCNR_MatSci	ITL/CTL
	Lecture Room B	**Lecture Room D**
Time	Moderator: Aaron Forster	Moderator:
1:30P	*Preetom Borah*: Optimization of thermal desorption direct analysis in real time mass spectrometry (TD-DART-MS) for the detection of illicit narcotics	*Carroll Reed, III*: Scan and Analysis of HTTPS Certificates Used in the .gov Domain
1:50P	*John Collin*i: Nanomechanical time-dependent properties of PEG Hydrogels	*Matthew Wilkes*: Developing a Mininet Test Suite for Software Defined Internet Exchange (SDX) Research
2:10P	*Jonathan Huff*: Software Development for a Precision Nanoindenter	*Ian Davila*: Test and Measurement of Software Defined Virtual Networks
2:30P	*Joseph Lagnese*: Analyzing the Analyzer: A Monte Carlo Investigation of X-Ray Diffraction Fits Generated by TOPAS5	*Jose de la Vega:* Test and Evaluation of Network Anomaly Detection Technologies
2:50P	*Matthew Bleakney*: Determining and comparing skeletal density of NIST RM-8852 from different gas measuring techniques/principles	*Aditya Dash*: Performance Monitoring and Instrumentation of Named-Data Networks
3:10P	**Break**	**Break**
	Moderator: Brandi Toliver, Managing SURF Director	Moderator:
3:20P	*Christine Plavchak*: Determination of 1H NMR spin diffusion coefficients via standard P3HT-PCBM bilayer films	*Rohan Tilva:* C-Force Enterprise: A Model-based Definition and Management of Cloud Metrics
3:40P	*Richard Wu*: Morphology and Miscibility: Characterizing A-B-A/B'-C Triblock-Diblock Copolymer Blends	*Joshua Massey*: C-Force Enterprise: Towards an Implementation of NCCP Cloud Metrics Model
4:00P	*Gordon McCann*: Simulation of Superquadric and Supertoroid Particles to Examine the Effects of Particle Shape upon Self-Assembly Behavior	*Matthew Landen:* Chaining the Cloud, The C-Force's Cryptographic Hash-Chaining Logging Approach
4:20P	*David Anderegg*: Developing a System to Encode Multicomponent Adsorption Isotherms for Standard Reference Data Use	*Samuel Cooper*: Detecting malicious users and compromised accounts using user behavioral models for the C-Force Enterprise's cloud service
4:40P	*Kailey Strack*a: Developing a System to Encode Multicomponent Adsorption Isotherms for Standard Reference Data Use	*Kelsey Fulton*: Unwinding the Runtime Stack: Application Runtime Analysis for Anomaly Detection Research
5:00P	**END**	**END**

SURF Colloquium: Wednesday, August 3, 2016 (Afternoon)

Parallel Sessions Agenda: EL and PML- Electrical Eng

	EL	PML-Electrical Eng
	Location: Heritage Room	**Location: Portrait Room**
Time	Moderator	Moderator: Joseph Kopanski, PML SURF Director
1:30P		*Firehiwot Warsa Gurara*: Magnetic Field Uniformity Through Pole Face Optimization
1:50P	*Malachi Yeh*: BIRDS: Quantifying Sustainability in Commercial Buildings	*Corey Rhode*s: Designing a Charge-Based Capacitance Measurement Circuit for Interfacing with an Atomic Force Microscope
2:10P	*Edward Hanson*: Community Resilience: Measuring Economic Benefits of Planning for Natural and Manmade Hazards	*Karl Montgomery*: Broadband Spectroscopic Characterization of Low-k Dielectric Thin Films for Micro- and Nanoelectronic Applications
2:30P	*Raef Youssef*: Implementing the ISO 15746 Standard and the Optimization Metamodel for Process Parameter Optimization	*Anthony Guo*: Metrology for Organic Spintronic Devices
2:50P	*Kevin Li*: Defining a Similarity Metric for Manufacturing Processes	*Theodore Nikolaitchik*: Molecular Interfaces and its Impact on Electronic Functionality
3:10P		*Colin Wade*: The electronic stability of polymer dielectrics for use in low temperature measurements of organic electronics
	Moderator:	Moderator: Darwin Reyes, PML SURF Director
3:20P	*Nathan Peterman*: Creating Design Allowables for Additively Manufactured Parts	*Lily Motabar*: 3D Printing Microfluidic Devices with Electronic Functionalities
3:40P	*Tawsif Siddiqui*: Schema and Ontology Development for the Additive Manufacturing (AM) Database	*Yasmine Kehnemouyi*: How to Produce a Microfluidic Device in No Time
4:00P	*April Nellis*: Verifying Analyses of Manufacturing Processes Using Predictive Models and Ontologies	*Michael Goebel*: Locking Lasers Using a Digital Servo
4:20P	*Vaughn Varma*: The Internet of Things on the Shop Floor: Design and Implementation of a Service-Oriented Architecture in Manufacturing Systems Utilizing B-SCADA's Status Enterprise	*Eileen Liu*: Using MATLAB in the Development and Optimization of Nanoscale Measurement Techniques
4:40P		*Theodore Zirkle*: Experiment Design to Analyze the Effect of Roughness and Machining Operations on Light-Based Three-Dimensional Coordinate Measuring Devices

SURF Colloquium: Thursday, August 4, 2016 (Morning)

Parallel Sessions Agenda: MML/NCNR-MatSci and ITL/CTL

	MML/NCNR-MatSci	ITL/CTL
	Location: Lecture Room B	**Location: Lecture Room D**
Time	Moderator: Guebre Tessema, National Science Foundation	Moderator:
9:00A	*Madeleine Pasco*: The effect of nanoparticle architecture and softness on the mechanical properties of the composite polymer	*Stephen Hockley:* Building a Cloud Forensic Reference Architecture: Leveraging AWS CloudTrail to Identify Forensics Artifacts.
9:20A	*Danielle Villa*: Neutron Scattering studies of the Crystal and Magnetic Structures of Molecular Magnets	*Daniel Vargas*: Forensic Analysis Automation: Determining Footwear Image Quality Using Machine Learning
9:40A	*Anthony Ayala*: Selective gas adsorption in metal organic frameworks	*Janelle Henrich:* Finding the Matching Pair: The Use of Graph Theory in Forensic Footwear Analysis
10:00A	*Douglas Scott*: Structural and Mechanical Characterization of HPMC/SDS Aggregation through Rheological and Neutron Scattering Measurements	*Sonny Aliakbar:* Can't Touch This: Usability of Contactless Fingerprint Acquisition Devices
10:20A	*Paul Neves*: Designing an AC Magnetic Susceptometer Measurement Technique in Conjunction with High Pressures and Low Temperatures in Neutron Beam Experiments	*Curtis Lamp:* Quantifying Latent Fingerprint Preprocessing
10:40A	Break	Break
	Moderator Name: Leonard Spinu, National Science Foundation	Moderator
11:00A	*Samantha Isaac*: Monte-Carlo Exploration of Focused Neutron Guide and Monochromator Geometries	*Ankur Patel:* Evaluation of a Plenoptic Camera for Capturing 3D Footwear Impressions
11:20A	*Daevin Hugh*: Characterizing and Verifying Parameters for Two New Mechanical Systems Through the Multiaxial Deformation of Automotive Sheet Metal	*Christopher Dare:* Latency of Lightweight Cryptographic Algorithms
11:40A	*Richard Leos Jr.*: Enhanced Safety Analysis Code Suits for the Reactor Design at NCNR	*Emily McGovern:* Analyzing the permutation testing methods of NIST SP 800-90B
12:00N	*Ryan Bonk*: Optimization Study on the Cold Neutron Source for a Proposed LEU Reactor at NIST	*Jose Rodriguez, Jr.*: Health Tests of Entropy Sources on Arduino
12:20P	*Ryan Fangmeyer*: System Control: Upgraded Refrigerator	*Ramo Collazo-Martis:* Strong Key Generation on Conventional Computer Systems Enabled by a Remote Entropy Source
12:40P		

SURF Colloquium: Thursday, August 4, 2016 (Morning)

Parallel Sessions Agenda: MML/NCNR-ChemBio

	MML/NCNR-ChemBio
	Location: Lecture Room A
Time	Moderator: Russ Johnson
9:00A	*Denis Routkevitch*: Analysis of metals in electronic cigarette vapor
9:20A	*Steven Knowlden*: Mercury Emissions: A Comparative Analysis of Mercury Generator Certifications, Past and Present
9:40A	*Anh Tran*: How Safe is Our Ginger? A Study of Arsenic Species in Standard Reference Material (SRM 3398) Ginger Rhizome
10:00A	*Abigail Lee*: Determination of Vitamin C in NIST Food-Matrix Standard Reference Materials
10:20A	*Imanuel Bie*r: Understanding the Effects of Spices in Homemade Explosives Detection by Ion Mobility Spectrometry (IMS)
10:40A	**Break**
	Moderator Name: Michael Halter
11:00A	*Ebony Cross*: Bioinformatic Analysis for the Standardization of Mouse Cell Line Authentication
11:20A	*Matthew Morse*: Automatically Generated Terminology and Scalable Webtools for Semantic Searching
11:40A	*Graham Rich*: Understanding the impact surface roughness has on gas adsorption
12:00N	*Ann Marie Martin*: Optimization of 3D Molecular Structures for the NIST Chemistry WebBook
12:20P	*Nimit Patel*: Optimization of 3-Dimensional Molecular Structures for NIST Chemistry WebBook
12:40P	*Mariya Shevchuk*: Optimization of 3-Dimensional Chemical Structures for NIST Chemistry WebBook

SURF Colloquium: Thursday, August 4, 2016 (Morning)

Parallel Sessions Agenda: EL and PML-Electrical Eng

	EL	PML-Electrical Eng
	Location: Heritage Room	**Location: Portrait Room**
Time	Moderator:	Moderator: Richard Steiner, PML SURF Director
9:00A	*Kirill Rebrov*: A Correction for Velocity Penetration Error at Immersed Boundaries in the Fire Dynamics Simulator (FDS)	*Claudia Gamble*: Testing Smart Watthour Meter Accuracy
9:20A	*Kenneth De Jesus Morales*: Towards a Robust Bench-scale Test for Predicting Smoldering Ignition of Residential Upholstered Furniture (RUF)	*Nathan Verrill*: Power System Synchrophasor Data Impairment using Labview
9:40A	*Muhong Han*: Fire-Blocking Performance of Laminated Barrier Fabrics	*Robert Davis*: Broadly Tunable, Narrow Linewidth Lasers
10:00A	*Bruk Haile*: Developing a database using GIS for extreme fire behavior	*Anton Vasilyev*: Evaluating Distortion Correction Methods for High-Resolution Digitizers
10:20A	*Eric Auth*: Wind and Separation Distance Effects on Fence Fire Spread in the Wildland Urban Interface	
10:40A	*Katrina Wakeman*: Alterting the Public in Community-wide Disasters: A Literature Review on Outdoor Warning Sirens	
	Moderator	Moderator: Dean Jarret
11:00A		*Sai Meghasena Chavali*: Measuring the wavelength of a cold neutron beam for a neutron lifetime experiment
11:20A		*Robert Buttles*: Automation of an Optical Pressure Standard: Dante's Divine Comedy of Pressure
11:40A		*Arlene Chiu*: Temperature Coefficients on Guarded Hamon Transfer Standards
12:00N		*Nhi Van Phan*: The Hadamard Transform Hyperspectral Image Projector
12:20P		
12:40P	**LUNCH**	**LUNCH**

SURF Colloquium: Thursday, August 4, 2016 (Afternoon)

Parallel Sessions Agenda: MML/NCNR-MatSci and ITL/CTL

	MML/NCNR-MatSci	**ITL/CTL**
	Location: Lecture Room B	**Location: Lecture Room D**
Time	Moderator: Dan Neumann	Moderator:
1:30P	*Aaron Schankler*: Refining a Markov Chain Monte Carlo Algorithm for Fitting Neutron Reflectometry Data	*Xinyu Xiong*: Access Control Rule Logic Circuit Simulation (ACRLCS)
1:50P	*Nathan Super*: BLAND UI: User Friendly Neutron Diffraction Analysis	*Zachary Ratliff:* Measuring the Combinatorial Coverage of Software in Real Time
2:10P	*Ian Hunt-Isaak*: Small Angle Scattering Calculator for Periodic Boundary Conditions.	*Myra Deng:* A Probabilistic Method for Counting the Number of Linear Extensions in a Partially Ordered Set
2:30P	*Hayley Boigenzahn*: Using Molecular Dynamics to Investigate the Structure of Polyelectrolyte Micelles	*Jane Pan*: Impact of Model Uncertainty on Statistical Inferences
2:50P	*James Gayvert*: Molecular Dynamics Study of the Conformational Properties of Polymers in an Explicit Solvent and the Identification of the θ-Temperature	*Jillian Kasner*: Simulation study of an automated threshold selection for Poisson process extreme value models
3:10P	Moderator:	
	Kathleen Mullin: Enabling Discovery of Materials Science Resources Through Robust Metadata Records	
3:20P	*Edward Nusinovich*: The application of data mining techniques for efficient material design	
3:40P	Lorelis Gonzalez Lopez: Using capillary force lithography to make oriented polymer nanogratings	
4:00P	*Ai Nguyen*: A performance of water and light: Characterizing water purification membranes using ellipsometry	
4:20P	*Atman Panigrahi*: Investigation of Salt Transport of Model Polymer Thin Films Via Electrical Impedance Spectroscopy	
4:40P	*Matthew Wade*: Calculation of Radial Distribution Functions using Histogram and Spectral Monte Carlo Methods on a Graphical Processing Unit	
5:00P	End	End

SURF Colloquium: Thursday, August 4, 2016 (Afternoon)

Parallel Sessions Agenda: Special Programs and CNST

	Special Programs	CNST
	Location: Heritage Room	**Location: Portrait Room**
Time	Moderator	Moderator: Vince Luciani
1:30P	*Joseph Emelike*: Golden Cross Section	*Arthur Sloan*: Self-Aligned Double Patterning as a Technique to Improve the Critical Dimension of i-Line projection lithography
1:50P	*Miriam Ekwuru*: Commercialization of Inventions in the Fields of Bio-Manufacturing and Medical Devices	*Mattie Watson*: Fabrication of Nano-scale High-Aspect-Ratio Structures through a Newly Devised Etching Process
2:10P	*Benjamin Resnick*: Marketing and Licensing of Microscopy Technology	*Jack Scaletta*: High-Q Surface Plasmon Resonator for Terahertz Time-Domain Spectroscopy
2:30P		*Gina Wong*: Controlling a nitrogen-vacancy center diamond to measure magnetic properties at the nanoscale
2:50P		*Gillen Beck*: Modeling of surface plasmon polariton coupling on a periodic grating and electro-optic polymer for faster spatial light modulation

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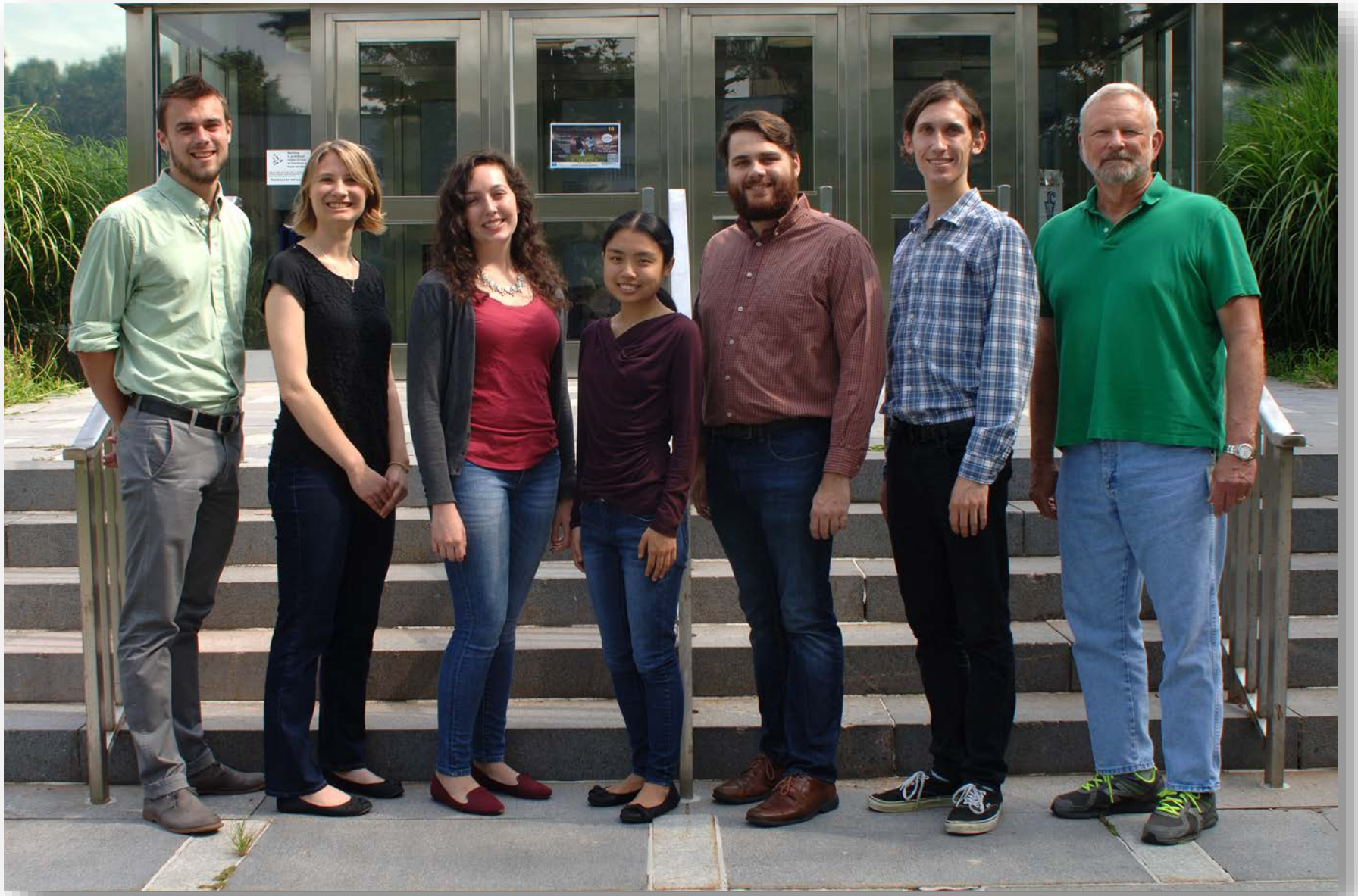

CNST

Center for Nanoscale Science & Technology (CNST)

Beck, Gillenhaal

Bourland, Kimberly

Scaletta, John

Sloan, Arthur

Watson, Martha

Wong, Gina

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Gillenhaal Beck		**Grant Number**	70NANB16H156
Academic Institution:	Washington and Lee University	**Major:**	Physics and Mathematics
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Graduate school for Applied Physics		
NIST Laboratory, Division, and Group:	Center for Nanoscale Science and Technology, Nanofabrication Research Group		
NIST Research Advisor:	Vladimir Aksyuk and Brian Roxworthy		
Title of Talk:	Modeling of surface plasmon polariton coupling on a periodic grating and electro-optic polymer for faster spatial light modulation		

Abstract:

Surface plasmon polaritons (SPPs) are optical-frequency electromagnetic excitations of free electrons in a metal, which can propagate along the metal-dielectric interface. With specific metal and dielectric geometries, we can create an SPP resonator, where the metal's permittivity and dielectric's refractive index influence the resonance frequency. When the wavelength of incident light matches the resonance, photonic energy is absorbed in exciting the SPP and there is a loss in the light's reflectivity. Therefore, the wavelength where this loss occurs can be manipulated by adjusting the dielectric's refractive index.

In many applications it is desirable to create dynamic, electrically controlled spatial patterns of light intensity or phase. This is commonly done with liquid crystals – dielectric materials with optical properties strongly dependent on applied electric field. These are widely used to form images on TV screens and to manipulate infrared optical signals in telecommunications switches, however they suffer from slow electro-optic response.

State of the art electro-optic (EO) polymer could be used to bypass this problem with a faster response time to voltage, while plasmonics can resonantly enhance the modulation strength. I have developed and numerically optimized a design for an EO plasmonic amplitude modulator, which operates on the coupling of SPP modes between a gold nanowire grating and a thin gold film, separated by a film of EO polymer. Modeling results indicate a strong plasmonic coupling between not only the film and wires, but also between pairs of wires themselves, providing for a system extremely sensitive to small changes in the polymer's refractive index. The combination of fast modulation at low applied voltage with a feasible nanofabrication process makes this system particularly promising.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Kimi Bourland		**Grant Number**	70NANB16H147
Academic Institution:	University of Colorado - Boulder	**Major:**	Chemical Engineering
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Center for Nanoscale Science & Technology, Electron Physics Group		
NIST Research Advisor:	Jabez McClelland		
Title of Talk:	Exploring Li-Ion Battery Materials with Focused Ion Beams		

Abstract:

Lithium-ion battery performance is limited, in part, by the ion-storage capacity of intercalation-based electrode materials like graphite and cobalt oxide. Electrodes based on materials that alloy with lithium, such as silicon and tin, can have large ion-storage capacities and serve as promising alternatives to pre-existing battery materials. However, lithium alloying materials suffer from a host of material fatigue problems during cycling that lead to rapid capacity loss. Improved understanding of these materials at the nanoscale will likely be required in the development of next-generation batteries, and this understanding will benefit from the creation of new analytical models and methods of investigating battery-relevant materials.

Our goal is to explore the lithium reaction front in tin at the nanoscale, using both experimental and theoretical models. To investigate the dynamics of the lithium reaction front in tin microspheres, we implement a novel lithiation technique using a lithium focused ion beam. This method allows for direct, spatial control over the lithium dose and can avoid the complications presented by solid electrolyte interfaces. Analysis of the reaction front involves cross-sectioning the tin spheres with a gallium focused ion beam in conjunction with imaging with a scanning electron microscope. Numerical modeling is used to relate our experimental results to several theoretical predictions. As a result of combining these experiments and models, our method will allow better understanding of how lithium behaves in tin, furthering efforts to create the next generation battery.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Jack Scaletta		**Grant Number**	70NANB16H142
Academic Institution:	Williams College	**Major:**	Physics, Theatre
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Center for Nanoscale Science and Technology, Energy Research Group		
NIST Research Advisor:	Amit Agrawal		
Title of Talk:	High-Q Surface Plasmon Resonator for Terahertz Time-Domain Spectroscopy		

Abstract:
The Terahertz frequency band lies between the microwave and infrared bands of the electromagnetic spectrum and is the subject of much current research. Terahertz radiation has a multitude of interesting properties, including being easily transmitted through many common materials, such as fabrics, rendering them transparent. In addition, much of the terahertz range of frequencies is at resonance with many molecular rotations, making it a highly effective way of obtaining information via spectroscopy. These properties make terahertz highly applicable in fields such as security systems, medical imaging in cancer research, astronomical molecular analysis, and more. However, there is a current dearth of technologies applicable to the terahertz range, as these frequencies are too high to be generated or detected by purely electronic or optical means. Terahertz time-domain spectroscopy has shown to be one of the few methods of successfully generating and detecting terahertz radiation, and as such uses terahertz to determine certain physical properties about the samples with which it interacts. In our research, we explore how the precision and Q-factor of measurements taken with time-domain spectroscopy can be improved using the surface plasmon resonance. In this project, we design a metal device consisting of multiple cups of various widths. Both photolithography and 3D polymer printing with metal deposition are employed to build these devices. Then, using a femtosecond laser with optical rectification to create terahertz pulses, we excite surface plasmons within the cups of the metal device. The plasmons resonate within the cup structure, which we then monitor by electro-optic sampling. We speculate that the resulting data will be in the form of an ultrahigh Q frequency spectrum typical of Fabry-Perot type resonators. If this is confirmed, this metal device could be used to improve the selectivity and precision of technologies that employ terahertz spectroscopy.

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NIST – Gaithersburg, MD
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Name: Arthur Sloan		**Grant Number**	70NANB16H133
Academic Institution:	Auburn University	**Major:**	Chemical Engineering
Academic Standing (Sept. '16):	Graduate School		
Future Plans (School/Career):	Attending Rice University to pursue a Ph.D. in chemical engineering		
NIST Laboratory, Division, and Group:	Center for Nanoscale Science and Technology, Nanofab Operations Group		
NIST Research Advisor:	Liya Yu		
Title of Talk:	Self-Aligned Double Patterning as a Technique to Improve the Critical Dimension of i-Line projection lithography		

Abstract:
This research aims to explore processing conditions and other parameters essential to utilizing self-aligned double patterning (SADP) techniques in the process flow for the NIST Nanofab i-line (365 nm) stepper. It also aims to reduce the overall number of processing steps for the SADP process. Photolithographic techniques have an inherent feature resolution limit, termed the critical dimension (CD), determined by the wavelength of light used and the optics of the processing equipment. For the i-line stepper, this limit is approximately 280 nm. Various techniques exist to circumvent this physical limit, usually involving the decomposition of the final pattern into multiple exposures. While techniques that break up the pattern into multiple lithography steps are versatile, they are vulnerable to alignment issues between individual exposures, and require additional intermediate processing steps, increasing the cost per device. SADP remediates the alignment issue by using a single mask to serve as a guide to deposit a spacer material. Removing the masking layer while leaving the spacer leads to an etch mask with double the feature density that can then be transferred to the substrate. For this research, photoresist layer was exposed with line patterns in various widths (300 nm to 1μm) on i-line projection lithography stepper and developed in tetramethylammonium hydroxide (TMAH) developer. Behaviors of two spacer materials, silicon nitride and chromium metal produced by physical vapor deposition, were characterized. The spacer material was deposited directly over the photoresist in varying thicknesses and subsequently etched back to form SADP spacers. Residual photoresist was removed using an acetone wash. A final plasma etch was performed to transfer the pattern onto the silicon substrate. Between each processing step, results were evaluated with scanning electron microscopy (SEM) to evaluate the effect of process parameters such as exposure energy, sputter time, spacer thickness, and etch time.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Mattie Watson		**Grant Number**	70NANB16H139
Academic Institution:	George Washington University	**Major:**	Mechanical Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	I plan to either pursue a graduate degree or go right into industry in with a nanotechnology or fluids field.		
NIST Laboratory, Division, and Group:	CNST, Nanofabrication, NanoFab Operations Group		
NIST Research Advisor:	Lei Chen		
Title of Talk:	Fabrication of Nano-scale High-Aspect-Ratio Structures through a Newly Devised Etching Process		

Abstract:

Deep silicon etching (DSE) is a critical process step in nano-fabrication. Nano-fabrication is key to the semi-conductor industry and creating computer chips. This process becomes more difficult and longer if it is used to produce a high-aspect-ratio (HAR) etch. This type of etch is the characterized by a large ratio of the height to the width. To achieve high-aspect-ratio nano-Si structures is challenging as it requires proper mask materials, high mask etching selectivity, and accurate control of the etching profile, angle and sidewall. Many approaches have been proposed and studied to fabricate HAR structures. The well-known processes include continuous cryogenic etching, alternating "Bosch" etching and atomic layer etching. However, those processes can require low temperature, cannot achieve smooth sidewall, or too slow in real application. We propose a new alternating plasma Si etching approach which separates the physical bombardment from the chemical reaction in the process. SF6 combined with C4F8, which have previously been shown to be a good etchant, alternates with Ar plasma and produces better results than the combining the three gases. By altering the plasma control parameters (gas flow, step time, upper and lower chamber power etc.), an optimized process is developed to achieve faster Si etching rate and better mask etching selectivity. Analysis of the results, which includes the etching rate, and the selectivity, are performed by scanning electron microscopy (SEM). Ultimately a clean high-aspect-ratio nano Si structure has been demonstrated. The newly developed Si etching process will be used for the applications such as making nanoelectromechanical systems and creating a diffraction grating for x-ray phase imaging.

SURF Student Colloquium

NIST – Gaithersburg, MD
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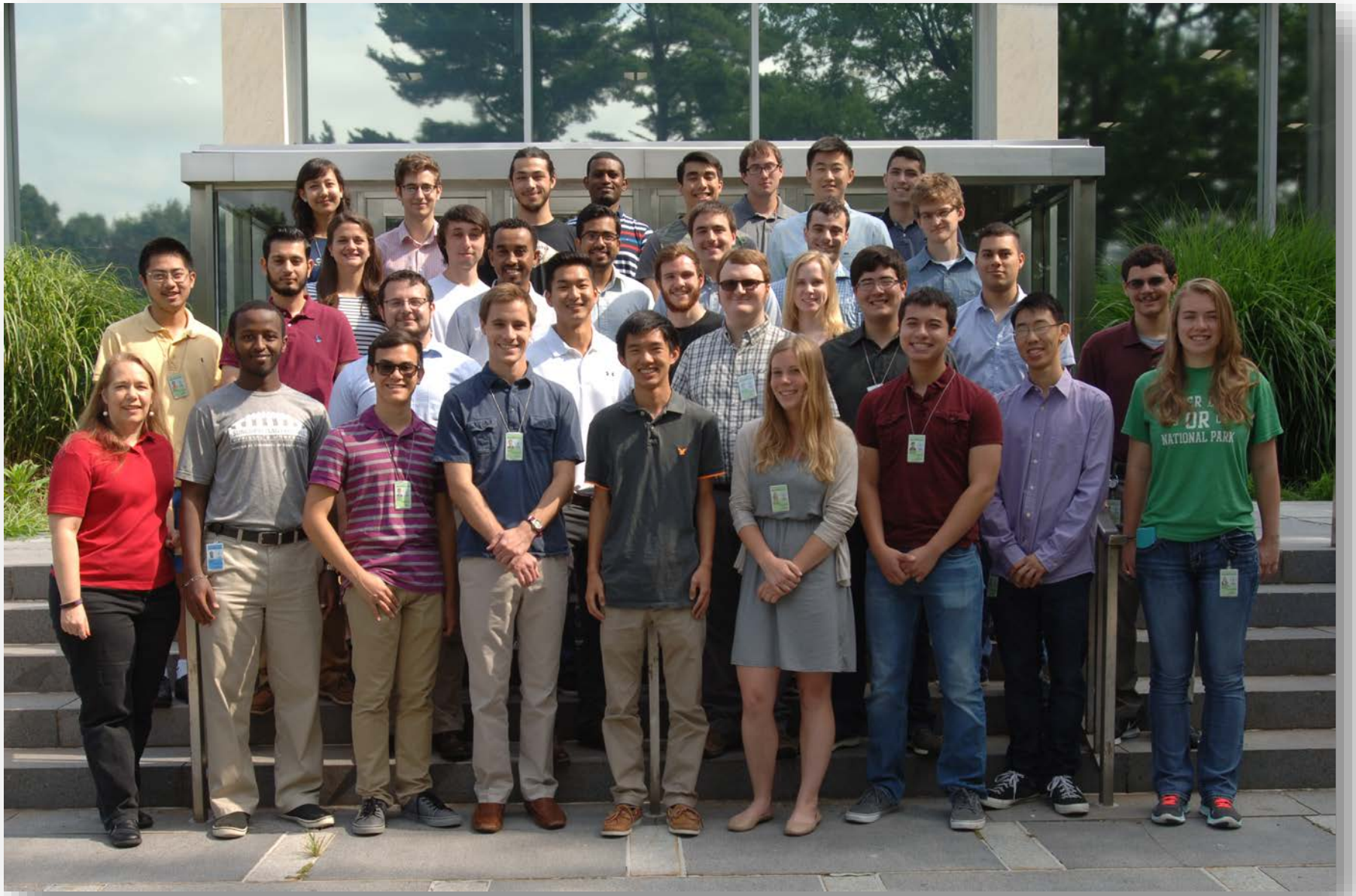
Name: Gina Wong		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland - College Park	**Major:**	Electrical Engineering, Physics
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Graduate school		
NIST Laboratory, Division, and Group:	Center for Nanoscale Science and Technology, Electron Physics Group		
NIST Research Advisor:	Dr. Robert McMichael		
Title of Talk:	Controlling a nitrogen-vacancy center diamond to measure magnetic properties at the nanoscale		

Abstract:

In the Nanomagnet Dynamics lab, we are developing precise measurements of magnetic fields near the surface of nanoscale magnets. Our two main challenges are (1) finding a sensor that is small enough to get close to the nanomagnets and (2) holding that sensor in a stable position. Nitrogen-vacancy (NV) centers, a type of defect in a diamond lattice, can function as precise magnetic field sensors. Not only are NV centers extremely sensitive to magnetic fields, but they can be created within nanometers of the diamond surface to perform nanoscale detection/imaging of magnetic fields.

My work focuses on the problem of sensor stabilization. I will discuss the use of a quartz tuning fork (QTF) in bringing an NV-center diamond to within nanometers of a sample surface. The effect of surface forces on the resonance frequency of a QTF can be used to determine its distance from a surface. My presentation will focus on how the piezoelectric properties of quartz crystal allow the QTF to be controlled to create an image of the surface with atomic resolution.

EL



Engineering Laboratory (EL)

Aboul-Enein, Omar

Auth, Eric

Caren, Stephen

De Jesus Morales, Kenneth

Goh, Justin

Haile, Bruk

Han, Muhong

Hanson, Edward

Hoddinott, Philip

Johnson, Theodore

Kamieniecki, Daniel

Kifle, Behailu

Krueger, Christina

Leader, Robert

Li, Kevin

McIntrye, Rachel

Mennu, Matlock

Nellis, April

Parsons, Matthew

Rebrov, Kirill

Seiler, Patrick

Siddiqui, Tawsif

Springer, Adam

Stoddard, Alexander

Super, Nathan

Varma, Vaughn

Wakeman, Katrina

Weaver, Samantha

White, Shawn

Winnard, Thomas

Yeh, Malachi

Youssef, Raef

Zhang, Tony

SURF Student Colloquium

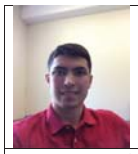
NIST – Gaithersburg, MD
August 2-4, 2016

Name: Omar Aboul-Enein		**Grant Number**	70NANB16H086
Academic Institution: Salisbury University		**Major:** Computer Science and Mathematics	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	I plan to cultivate interests in computer vision, distributed computing, and cybersecurity further as I pursue a Master's degree in computer science. In addition, I plan to pursue my enthusiasm in research by exploring opportunities with agencies such as the NSA, Department of Defense, or NIST itself.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Manipulation and Mobility Systems Group		
NIST Research Advisor:	Roger Bostelman		
Title of Talk:	Augmented Reality Marker Tracking for Multi-Robot Registration		

Abstract:
In pursuit of the NIST mission to provide information on emerging markets, the Engineering Laboratory is investigating topics in smart manufacturing to develop performance knowledge pertaining to various robotic fields. A subset of this research involves developing test methods for "mobile manipulator" robots. Mobile manipulators refer to a range of robotic systems that feature two main components, a mobile robot or base and an onboard robot arm or manipulator, that collaborate within industrial environments. The mobile base, such as a traditional Automatic Guided Vehicle (AGV), is used for autonomous navigation and docking. This capability can be used to reposition an onboard manipulator arm to perform automatic assembly tasks. The ASTM Committee F45 on Driverless Automatic Guided Vehicles was formed, in part, to define test methods for these complex systems. In developing new test methods for this committee, we seek to measure the performance of mobile manipulator robots for industrial applications and thus provide rapid, economical smart manufacturing solutions.

Previous research for these test methods focused on the performance measurement of the mobile base to navigate and dock the manipulator. Implementation of this test required the development of inter-system communication between the mobile base and onboard manipulator. A NIST artifact, the Reconfigurable Mobile Manipulator Artifact (RMMA), is used to assess the mobile manipulator's docking and navigation capabilities. Reflective targets installed on the RMMA were used in conjunction with a retroreflective laser sensor mounted on the manipulator to test the mobile manipulator position and orientation (pose). However, the inability of the mobility system to accurately dock with the RMMA and communicate pose data to the robotic arm restricted the possible testing scenarios. A solution to this problem included the integration of an open source augmented reality toolkit, Alvar AR. The AR software toolkit, which is designed to develop applications that overlay virtual images on 2D fiducials, was essentially repurposed into a marker-based tracking system by recording the pose of markers fixed to the RMMA.

Current advancements in the mobility system allow pose information to be communicated between the two different robots with ease. However, improvement in manipulator registration is desired such that targets can be detected rapidly despite known uncertainties in mobile base docking. For this test method, we adapt AR marker tracking to first calibrate the marker, camera, and laser offset to the camera, and then rapidly position the laser to detect assembly targets. The development of this solution involved the consolidation and integration of existing networks and hardware with the ARToolkit SDK for Windows, as well as the calibration of the augmented reality tracking system. Lastly, while this test method is applied to improve the registration of traditional systems, registration is also investigated for use with advanced, autonomous, mobile manipulators to solve similar communication and registration problems.



SURF Student Colloquium

NIST – Gaithersburg, MD
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Name: Eric Auth		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland College Park	**Major:**	Fire Protection Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Master's in Fire Protection Engineering from University of Maryland College Park		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Wildland Urban Interface Group		
NIST Research Advisor:	Rik Johnsson		
Title of Talk:	Wind and Separation Distance Effects on Fence Fire Spread in the Wildland Urban Interface		

Abstract:
The fires that cause the most property damage annually are those that make their way to or through intersections between forests and developed areas. These zones, collectively known as the Wildland-Urban Interface (WUI), contain 46 million structures which are put at risk every year. While much is known about home ignition due to direct flame contact and radiation, firebrands and nearby auxiliary structures also play a large role in the ignition of structures and are becoming the main topic of research with regards to the WUI. These auxiliary structures include woodpiles, decks, and fences which allow the fire to spread to homes more easily.

This summer, experiments were performed to study the effects of wind speed and separation distance from fence to structure upon flame spread to the structure. The test assembly consisted of a wooden privacy fence (with or without mulch underneath) which was oriented perpendicular to a shed, and a wind machine operated at 20 mph (9 m/s) and 30 mph (13 m/s) to simulate similar WUI fire wind conditions, in a direction parallel to the fence. A bi-directional probe was located 4 ft (1.2 m) in front of the test assembly to measure the wind speeds and determine the wind's velocity profile. Separation distance between the fence and the shed was varied to study the effect of distance on structure ignition. The results from these tests will be used to provide technical foundation for mitigation strategies in WUI fire prone regions.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: Stephen Caren		**Grant Number**	70NANB16H125
Academic Institution: Wayne State University		**Major:** Chemical Engineering	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	I intend to either apply for graduate school and research sustainability or work for TARDEC, eventually attaining a Master's degree.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Polymeric Materials Group		
NIST Research Advisor:	Lipiin Sung		
Title of Talk:	Artificial Sunny Days: Impact of Temperature on Polyethylene Photodegradation under Accelerated Weathering		

Abstract:
Polymeric materials exposed to weathering conditions such as solar ultraviolet (UV) radiation, heat, and moisture degrade and change their chemical and physical properties. Ductile polymers like polyethylene will become brittle after prolonged exposure to high temperature and radiation through thermolytic and photolytic degradation processes. Understanding the effects that these weathering parameters have on the speed of degradation is paramount to creating models for predicting property changes.

For this experiment, polyethylene samples were exposed in an accelerated weathering environment at 40°C and 50°C (100% UV intensity, and 0% relative humidity) by utilizing the NIST SPHERE exposure device (Stimulated Photodegradation via High Energy Radiant Exposure). Chemical and mechanical changes were characterized at different exposure times. Mechanical properties were measured via tensile test and chemical changes were monitored via FTIR-ATR (Fourier transform infrared spectroscopy – attenuated total reflection). The results at higher temperature were compared to the previous study at 30°C exposure conditions as well as to outdoor weathered samples.

Preliminary results showed that the higher temperature the higher degradation rate in both chemical and mechanical properties. Temperature dependence of the degradation behavior of polyethylene will provide a key insight of degradation kinetics and mechanism and will be included in the weathering database for service life prediction of polymeric systems.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: Kenneth De Jesus Morales		**Grant Number**	70NANB16H161
Academic Institution: University of Puerto Rico		**Major:** Mechanical Engineering	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Master Degree of Biomedical Innovation and Development (MBID), at Georgia Institute of Technology		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Flammability Reduction Group		
NIST Research Advisor:	Mauro Zammarano & Shonali Nazare		
Title of Talk:	Towards a Robust Bench-scale Test for Predicting Smoldering Ignition of Residential Upholstered Furniture (RUF)		

Abstract:
Residential upholstered furniture (RUF) is the single largest cause of civilian deaths in U.S. home fires (about 25%) with an annual estimated average of about 600 deaths, 9000 fires, 1100 injuries and $600 million direct damage. RUF fires (fires where RUF is the primary item contributing to fire growth) can be initiated by smoldering material (e.g., cigarettes) and open flames (e.g., candles). Smoldering is a non-flaming form of combustion that poses a severe fire hazard due to the potentially lethal amount of toxic carbon monoxide released, and the transition from smoldering to flaming. Surprisingly, more than half of deadly RUF fires are initiated by smoldering material. In the US, the smoldering propensity of RUF is assessed by bench-scale tests (Cal TB117-2013, ASTM E1353, and NFPA 260) that are all based on an identical test configuration. Unfortunately, we have found that these tests may not reliably predict the smoldering propensity of actual furniture. The Flammability Reduction Group at NIST has proposed a modified bench-scale test to address this issue.

In this work, we compared the smoldering behavior of RUF materials measured by the current bench-scale test, the proposed NIST modified bench-scale test and large-scale mockup tests. In particular, this project focused on processing and analyzing smoldering data collected in the large-scale mockup tests. Data processing included: synchronization of multiple point-of-view videos with infrared videos to investigate transition from smoldering to flaming, temperature profiles in the foam and fabric, heat release rate and gas analysis. These results show that the modified bench-scale test is a more robust predictor, as compared to the current bench-scale test, for the likelihood of smoldering ignition and transition-to-open-flame in the large-scale mockups.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: Justin Goh		**Grant Number**	70NANB16H131
Academic Institution: University of Maryland College Park		**Major:** Mechanical Engineering **Minor:** Technology Entrepreneurship	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	After getting my bachelor's degree, I plan on working for a big tech company developing robotic systems and starting my own business developing robots.		
NIST Laboratory, Division, and Group:	Engineering Lab, Intelligent System Division, Manipulation & Mobility Systems Group		
NIST Research Advisor:	Dr. Karl Van Wyk		
Title of Talk:	Simulation Assisted Robot Hand and Arm Programming for Planning and Simplifying User Experience		

Abstract:
With recent advances in robot technology, the number of robotic hands has grown. These hands are not your run-of-the-mill pneumatic grippers. They are bio-inspired in terms of their dexterity and sensing capabilities. Their adaptability and flexibility in manipulating different objects lowers the overhead cost associated with end-of-arm tooling, which makes them a viable option for small and medium manufacturing companies compared to conventional grippers or proprietary tooling interfaces. In support of this technology, the Manipulation & Mobility Systems Group at NIST is working on developing test metrics and benchmarks to help quantify the performance and advancement of robot hand technology. In addition, integration of robot hand technology within robotic systems is aided with the use of simulation environments. In this case, a simulation will be created using Robot Operating System (ROS) and Gazebo.

ROS is a flexible framework for writing robot software with a collection of tools, libraries, and conventions, which aim to simplify the task of creating complex and robust robot behavior across a variety of robotic platforms. Gazebo, used by DARPA and many other institutions and laboratories, is a simulator that has a robust physics engine, high quality graphics, convenient programmatic and graphical interfaces, and the capability to accurately and efficiently simulate populations of robots in complex indoor and outdoor environments.

The simulation will be a two-way street for communication. Utilizing ROS' subscriber (receiving data) and publisher (sending data) capability and its integration with Gazebo, we will be able to send the joint states of any robot arm or hand we have available in the lab to Gazebo via TCP/IP (Transmission Control Protocol/Internet Protocol). The same can be done in reverse to control the robot in real life via sending command joint positions by manipulating the model in Gazebo. The latter will be used to test planning algorithms. Grasp and path planning are an important part of the development of robotic hands because it automates the process for grasping a wide variety of objects in a high degree-of-freedom command space, which simplifies the programming experience for the end user.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: Bruk Haile		**Grant Number**	70NANB16H128
Academic Institution: University of the District Columbia		**Major:** Information Technology	
Academic Standing (Sept. '16):	Graduated college in Spring 2016		
Future Plans (School/Career):	Graduate school		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Wildland Urban Interface Group		
NIST Research Advisor:	Dr. Kathryn Butler		
Title of Talk:	Developing a database using GIS for extreme fire behavior		

Abstract:
Extreme fire behavior results when many of the elements of the fire environment interact to cause the rate of spread of the fire to increase by sixty times or more. Situations within which abundant fuels with sufficiently low moisture values are located on a steep slope and combine with robust winds and unstable atmospheric conditions will almost always result in extreme fire behavior. Each of these individual conditions will probably increase fire intensity; therefore, when all of these conditions occur at a similar time, the potential danger will increase considerably. Extreme fire behavior is resistant to direct fire suppression techniques, and typically involves one or more of the following characteristics: high rate of spread and frontal fire intensity, crowning, prolific spotting, presence of large fireplace whirls, and a well-established convective column. The objective of this project is to generate a database of extreme fire events, including location, dates, fire characteristics, and conditions contributing to the fire behavior. Geographic Information System (GIS) software will be used to map, display, and analyze data on regional and national scales.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Muhong Han		**Grant Number**	70NANB16H082
Academic Institution: East Carolina University		**Major:**	Engineering (biomedical), Physics
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Appling to George Tech for graduate school with a master degree in biomedical innovation and development.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Flammability Reduction Group		
NIST Research Advisor:	Shonali Nazare, Mauro Zammarano		
Title of Talk:	Fire-Blocking performance of laminated barrier fabrics		

Abstract:
A promising approach for reducing flammability of residential upholstered furniture (RUF), without adding flame retardants either to the flammable flexible polyurethane foam (FPUF) cushioning or to the cover fabric (CF), is to incorporate a fire-blocking barrier fabric (BF). Fabric lamination is a process of bonding two or more fabrics or flexible materials with diverse functionalities to produce a multi-functional product with desired performance properties. Lamination of BF to the CF also eliminates the need for sequential upholstering of fabric layers, thereby reducing the cost of labor. Moreover, fabric lamination extends the durability as it reduces the friction that occurs between the two fabrics if they were not adhered.

Three different types (knitted, woven and nonwoven) of commercially available BFs were laminated to three types of cover fabrics with varying physical properties. Thermal protective performance of laminated BFs was assessed using cone calorimetry data. Composite specimen comprising FPUF covered with laminated BFs were exposed to external incident heat flux of 35 kW/m^2 in a cone calorimeter. The fire-blocking effectiveness of laminated BFs was assessed by comparing heat release rate and mass loss data for specimens with and without laminated BFs. The differences in the shape of heat release rate curves and visual observations during the cone calorimetry experiments have been be used to differentiate the fire-blocking effectiveness of laminated BFs. The results indicate that the protective performance of laminated BFs is largely influenced by the structure of the barrier fabric. Gas permeability, which is mainly determined by the structural configuration of the BF, appears to be the key property in preventing the FPUF volatiles from coming in contact with heat and/or flames.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Edward Hanson		**Grant Number**	70NANB16H159
Academic Institution:	University Maryland Baltimore County	**Major:**	Computer Engineering
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	PhD in Computer Engineering. Interested in working in industry after contributing through research.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Applied Economics Office		
NIST Research Advisor:	Dr. Jennifer Helgeson		
Title of Talk:	Community Resilience: Measuring Economic Benefits of Planning for Natural and Man-made Hazards		

Abstract:
Disasters of all varieties can cause devastating damage to community infrastructure. Measures are often taken to reduce the negative impacts of such disasters. However, there is strong uncertainty around when disasters may occur for certain hazard types. Infrastructure within a community is a system of systems; if there is failure in one part, it is likely that the entire system will be disrupted. For this reason, community resilience planning should take place ahead of time; vulnerable structures should be properly reinforced against potential hazard events. First costs associated with such preparedness may be expensive; however, considering the lifecycle costs can make resilience projects more financially feasible.

Whenever a community decides to increase its resilience capacity there are clear benefits should a disaster occur. However, there are plenty of *co-benefits* that may be the product of increased community resilience even when a disaster has not yet occurred. Such co-benefits are rarely considered due to difficulty in valuing and quantifying indirect benefits. Certain co-benefits, such as reduced commute-time upon the creation of a new bridge, offer clear community benefits and should be considered in the disaster preparedness decision-making process.

The purpose of my project is to develop a tool that could produce a meaningful report on the benefits and costs of implementing several potential plans to improve resilience in comparison to the base case (i.e., taking no planning action). I have utilized NIST's *Economic Decision Guide (EDG)* to program a tool that can accept both quantitative and qualitative input from a user and calculate present expected values for alternative community resilience plans. The program presents the user with information about the steps in the *EDG* by providing information on how the implementation of the *EDG* may benefit a given community. In addition to this tool, I also aim to find academic and policy material related to the topic of the *Resilience Dividend*, the state in which co-benefits arise from implementing a resiliency plan, even when a disaster is not imminent. Development of an annotated bibliography on the subject will help further the research program on this currently under-researched area.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: Philip Hoddinott		**Grant Number**	70NANB16H088
Academic Institution: Rensselaer Polytechnic Institute		**Major:** Mechanical Engineering	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Graduate School in Mechanical or Aerospace Engineering		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Energy and Environment Division, Mechanical Systems and Controls Group		
NIST Research Advisor:	Glen Glaeser and Amanda Pertzborn		
Title of Talk:	Design and Construction of Intelligent Building Agent Laboratory		

Abstract:
To achieve the goal of a net zero energy building, energy consumption must be significantly reduced. At NIST the Intelligent Building Agents Project (IBAP) will lower energy consumption with the implementation of Intelligent Software Agents in commercial buildings. These Agents optimize building control systems by implementing distributed decision making to lower energy use.

The Intelligent Building Agent Simulation Program (IBAS) has already been created, and a lab for IBAP is currently under development. The lab has two systems; water and air. The air system emulates a building. The water system emulates a cooling plant for the building. The focus of my project has been working on the air system. The air system boasts over 80 sensors and a mile of wire. Careful planning went into the design and construction of the wire tracks to preserve the lab's modularity. By tracing the wire's path from the sensors to the data rack a "subway map" was created. This map was then used to install the wire tracks and run the wires inside those tracks. Sensors, including flow meters and Resistance Temperature Devices were installed to monitor the air system.

The air system uses dampers to control flow inside the ducts. Actuators that move were installed and control wired was connected to the data racks. One potential danger is the operation of fans with no flow path to the outside. This would over pressurize the ducts, presenting a danger to equipment and personnel. A safety program was written in LabVIEW to control flow paths. Part of this project was developing the programs that ensure safe operation of the air system.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Theodore Johnson		**Grant Number**	70NANB16H077
Academic Institution: Georgia Institute of Technology		**Major:** Electrical Engineering	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Research and Development in the field of Electrical Engineering		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Systems Integration Group		
NIST Research Advisor:	Nicholas Dagalakis		
Title of Talk:	Control System Implementation for Motorized Dynamic Bending and Calibration Machine		

Abstract:
The movement of manufacturing to countries featuring labor with low hourly wages over the last fifteen years has motivated the development of a new generation of industrial robots that can work side-by- side with human workers. This has created a new technology of Human-Collaboration-Robotics, which combines the intelligence and dexterity of humans with the strength, repeatability and endurance of industrial robots. Since most robots are powerful programmable moving machines, the safety of workers working around these robots has become a top priority for safety standards development that will provide guidance for the development of a comprehensive risk assessment of the robot arm, its tools, its controller, and the whole operating workspace where humans might be present. We are using bio simulant materials for the construction of disposable Human-Collaboration- Robotics safety testing artifacts. These testing artifacts will make possible the measurement of damage when humans and robots come into contact and the severity of injuries caused by robot static and impact pressure. In order to test and calibrate these artifacts we have constructed several simple and inexpensive testing machines, which simulate impact events and measure the mechanical properties of the artifact. The Dynamic Bending and Calibration Machine (DyBeCaM) simulates the application of programmable speed profile bending loads to human bio-simulant bone artifacts. The subject of this project is to create a control system and computer interface for a motorized version of the DyBeCaM (MoDyBeCaM) that would be able to control the instrument as well as record and analyze data about its movement.

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NIST – Gaithersburg, MD
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Name: Daniel Kamieniecki		**Grant Number**	70NANB16H102
Academic Institution: Stevens Institute of Technology		**Major:** Mechanical Engineering	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	A career in Computer Numerical Control (CNC) and robotics.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Inorganic Materials Group		
NIST Research Advisor:	Scott Jones		
Title of Talk:	3D Printing Cement: Characterization of printable cement pastes		

Abstract:
Additive manufacturing processes, specifically 3D printing, are increasing in popularity as the required hardware and software become more accessible. 3D printing cement is an attractive manufacturing process for geometrically complex structures that cannot be easily produced using conventional formwork methods.

An existing paste printer prototype, which employs the CNC capabilities of a small scale polymer 3D printer, was upgraded to a state of functionality. Cement paste is extruded via syringes through a nozzle, and is deposited layer by layer to build a three dimensional object. Although both printing parameters and material properties affect the ability to print, only the material properties were explored in this experiment. Several different cement pastes were mixed with limestone powders of varying particle sizes and high range water reducing agent. A water to solids ratio of 0.22 was kept constant throughout. The "printability" of each mixture was assessed using a challenging test print (a tall, thin wall) and a print performance rubric. Material flow behavior of each paste was measured using a rheometer.

Data from the rheometer was analyzed for yield stress, thixotropic behavior, and other viscoelastic properties. It was found that a specific range of yield stresses is optimal for printing. The mix with the best performance over a long period of time is a 25:50:25 proportion 16 µm limestone:cement:2 µm limestone by mass. The experiment helped develop a relation between paste yield stress and printability. Measurements and findings from the small printer provide insight and possibly scalable relationships to large scale cement printing.

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Name: Behailu Kifle		**Grant Number**	70NANB16H128
Academic Institution: University of the District Columbia		**Major:** Civil Engineering	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Pursue a graduate degree in Structural Engineering		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Inorganic Materials Group		
NIST Research Advisor:	Paul Stutzman		
Title of Talk:	Phase Analysis of Portland Cement Clinker by Scanning Electron Microscopy and X-Ray Powder Diffraction		

Abstract:
Concrete consumption per capita is second only to water with hydraulic cements as the "glue" that hold the aggregates of concrete together. Cement is composed of ground clinker and limestone, with gypsum added to control setting. Clinker is a sintered product from a mixture composed of ground limestone, sandstone, shale and iron, heated in kiln to 1700 °C to form agglomerates up to the size of a softball. Process control in cement manufacture requires routine testing of the clinker. The NIST Standard Reference Materials (SRM) Portland Cement Clinkers are used to develop and evaluate methods of quantitative phase analysis. They have been useful in testing laboratory analysis protocols and have assisted in the development of ASTM standard tests for microscopy and XRD.

As the SRM clinkers approach the initial estimate of their shelf life, an assessment of the composition and texture is necessary to make a decision on extending their life or replacement. Microscopy of Portland cement clinker provides a visual identification of the phase components as well as their size and distribution; useful information for monitoring kiln conditions in cement production. A set of high-resolution backscattered electron and X-ray images by scanning electron microscopy (SEM) are obtained from individual cement clinker particles. These images are evaluated for textural changes in the clinker and subjected to image processing and analysis to quantify the mass fractions of the components. The phase constituents, texture, structure, and distribution of the phases in microstructure of the clinker are digitally traced and extracted for measurement of area and mass fraction making quantitative microstructure imaging a practical method of performing phase analysis.

A set of complimentary X-ray powder diffraction (XRD) data provides a separate qualitative and quantitative phase assessment of the clinker. Applying both SEM and XRD methods to characterize a clinker can often provide a more complete and accurate analysis of the phase abundance.

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Name: Christina Krueger		**Grant Number**	70NANB16H131
Academic Institution: University of Maryland College Park		**Major:** Mechanical Engineering	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	A career in applied engineering		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Production Systems Group		
NIST Research Advisor:	Jarred Heigel		
Title of Talk:	Seeing between the lines: Layerwise imaging for metal additive manufacturing		

Abstract:
Additive Manufacturing (AM) processes build parts layer by layer using a variety of materials, including metals. Metal AM constructs each layer employing several techniques such as: powder bed fusion (PBF), which melts each metal powder layer often with a laser, and binder jet printing, which temporarily fuses the metal powder until it is sintered during post-processing. This technology has the potential to revolutionize the manufacturing industry; however, before widespread adoption, users must have confidence that every part is created as expected. This requires a combination of pre-process modeling, process monitoring, and post-process analysis. One step towards this goal is to develop a reliable layerwise defect detection system to identify possible defects during the printing process.

This project utilizes a high resolution camera (1.67 μm/pixel) that is automatically triggered to capture images before and after each printed layer. The imaging system combines an adaptable LabVIEW program for image acquisition with two hardware assemblies customized to image a commercial binder jet printer and a commercial power bed fusion system. The detailed designs of the imaging system setups and example results of layerwise imaging trials will be presented. This system creates a platform for automatic defect detection and supports current research that benefits from layerwise imaging.

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Name: Robert Leader		**Grant Number**	70NANB16H079
Academic Institution: Arizona State University		**Major:** Aerospace Engineering (Aeronautics)	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Graduate School at Arizona State		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Energy and Environment Division, Mechanical Systems and Controls Group		
NIST Research Advisor:	Natascha Milesi-Ferretti		
Title of Talk:	Tools for the Ongoing Commissioning of Buildings		

Abstract:
Commissioning building HVAC (Heating, Ventilation, and Air Conditioning) systems continuously, beyond the initial and annual inspections, can have significant positive impacts on energy usage, ease-of-use for operators and occupants, and equipment life. To accomplish this, one monitors various components of an HVAC system which includes devices such as sensors, pumps, motors, controllers, etc. and compares the performance of the devices and outputs to what the operation documentation describes as well as logical principles or "expert rules" e.g., the Cooling Valve should not open when the Air Handling Unit is in Heating Mode. If this comparison yields a fault, one would then want to discover its source and attempt to fix the problem.

Here at NIST, a computer program is being developed to monitor these building HVAC systems, analyze the data for faults and present them, and perform functional tests on individual components and systems. The software is currently in its proof-of-concept phase and thus its capabilities and efficiency are being tested and developed.

One part of my role in this research project has been to validate the capabilities of the analysis software as well as use it to monitor the HVAC performance of a real building, the Performing Arts Center at Montgomery College. Thus far, the program has successfully been used to monitor hundreds of relevant devices on the Montgomery College server, plot relevant data over a span of several months, and identify numerous operational faults. This process has shown several issues with the operations at the Performing Arts Center, has revealed several holes in the control logic, and has led to numerous insights in how to improve the software's usefulness and accuracy. The detailed findings of this passive analysis of both the building and the software are discussed in this talk. My other role in this research has been to develop scripts to test the functional performance of individual components- based on tests used by actual commissioning agents- using the testing module environment which is part of the software package. The success of this emulation and suggestions for future expansion of features are discussed in this talk as well.

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Name: Kevin Li		**Grant Number**	70NANB16H131
Academic Institution: University of Maryland College Park		**Major:** Mechanical Engineering	
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	I am starting research in tactile sensing and planning on pursuing graduate studies in electrical engineering.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Life Cycle Engineering Group		
NIST Research Advisor:	William Z. Bernstein		
Title of Talk:	Defining a similarity metric for manufacturing processes		

Abstract:
Manufacturing taxonomies and accompanying metadata of manufacturing processes have been catalogued both in reference books and databases online. However, such information remains in a form that is uninformative to the various stages of the product life cycle, including the design phase and manufacturing-related activities. This challenge lies in the varying nature in how data is represented, such as through words, a single value, or a range of values. The ASTM E3012-16 (Standard Guide for Characterizing Environmental Aspects of Manufacturing Processes) standard has formally characterized sustainability information of manufacturing processes through Unit Manufacturing Process (UMP) models. A web-based repository is under development to curate a set of such models to conduct further analysis on the processes. In this project, we apply widely accepted similarity measures that use edge-based, node-based (Information Content), and hybrid approaches to a set of manufacturing processes. Here, we develop a measure of similarity to the processes given specific attributes such as workpiece material, feasible tolerance ranges, and possible geometric properties of the product. To judge the effectiveness of these metrics, we apply permutations of them to a case study using several UMP models, i.e., drilling, milling, and reaming, that were created based on the E3012-16 standard. By experimenting with different metrics, we generalize a distance measure that effectively captures similarity between two UMPs. By linking entities within a manufacturing repository, we open up the possibility to connect the design and manufacturing phases to aid decision makers and designers. This work will eventually contribute to the development of interactive interfaces that reflect the breadth and depth of content in the UMP repository. Interfaces such as an interactive and a visual catalog can help identify alternative paths towards creating a product that can be optimized based on various performance metrics, including throughput, environmental impact, and cost.

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Name: Rachel McIntyre		**Grant Number**	70NANB16H131
Academic Institution: University of Maryland College Park		**Major:** Mechanical Engineering	
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	Finish Bachelor's Degree and pursue Graduate School		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Energy and Environment Division, Heat Transfer and Alternative Energy Systems Group		
NIST Research Advisor:	Behrang Hamadani and Brian Dougherty		
Title of Talk:	Temperature Dependent Measurements of Photovoltaic Solar Cells		

Abstract:
The photovoltaic (PV) industry has been growing. In 2015, 7.5 gigawatts of solar power were installed, which puts the total capacity installed at 29 gigawatts. About 25% of all solar power was installed last year. Greater emphasis has now been placed on PV module performance because with such a big installed volume, even a small percentage error in performance predictions can have a huge impact on the magnitude of generated power and its supply to the electric grid. Temperature has been shown to significantly affect the performance of photovoltaic cells, with higher temperatures generally resulting in lower electrical output from installed PV modules.

This work quantitatively explores the effect of temperature on various solar cell parameters, including open circuit voltage and short circuit current, which are important performance indicators. First, a solar simulator was used to record the effect of temperature on solar cell parameters under a broadband light source similar to the spectrum of the sun. Then, temperature-dependent spectral effects were examined using a monochromatic light emitting diode array (LEDs) consisting of 10 or more LEDs. These results indicate that the short circuit current in silicon-based solar cells showed the most temperature sensitivity in the near infrared region close to the maximum peak sensitivity of the solar cells.

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Name: Matlock Mennu		**Grant Number**	70NANB16H092
Academic Institution: University of South Florida		**Major:** Mechanical Engineering	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	I plan on attending graduate school for aeronautical engineering after finishing Bachelor's Degree in Mechanical Engineering. After finishing graduate school, I hope to work at a leading commercial airplane manufacturing company.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Production Systems Group		
NIST Research Advisor:	Greg Vogl		
Title of Talk:	Sensor-Based Diagnostics of CNC Linear Axes		

Abstract:
Computer numerical control (CNC) machine tools are essential tools in the manufacturing of various components in the automotive and aircraft manufacturing industry. Thus, degradation of machine tool linear axes has a huge impact on the quality of parts manufactured through this process. Billions of US dollars are lost every year due to degradation of machine tools during production. Currently, there are direct methods of measuring geometric errors using laser-based and other standard methods. However, these methods are time-consuming and complicated for many users. In addition, such methods halt production, which usually equates to lost revenue, so manufacturers prefer not to shut down their machines for tests. Therefore, this project focuses on using an inertial measurement unit (IMU) with relatively inexpensive sensors for measuring changes in geometric errors of linear axes efficiently and with sufficient accuracy. The IMU-based method has been tested with much success on a linear axis testbed. Now, a smaller IMU is being set up for placement and practical usage on machine tools.

The linear axis testbed relies on acquiring axis position data from the motor encoder in the system. The main challenge was to derive nominal position data from an accelerometer rather than relying on other sources, so that the IMU can be placed in a "plug and play" fashion on any machine tool without needing to acquire controller position data. This process involved writing MATLAB functions that can derive position data from acceleration data from the accelerometers in the sensor box. Once a robust method was developed, the estimated positions were compared with the measured positions (from the testbed encoder) to determine the method accuracy. After the accuracy was determined to be sufficient for analysis purposes, the function was integrated into the main analysis code that estimates linear axis errors as a function of nominal axis position. Finally, metrics were tested for their ability to distinguish various level of degradation from the linear axis error motions.

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Name: April Nellis		**Grant Number**	70NANB16H131
Academic Institution: University of Maryland College Park		**Major:** Applied Mathematics	
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	I plan to pursue graduate studies in mathematics.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, System Integration Division, Systems Engineering Group		
NIST Research Advisor:	Peter Denno		
Title of Talk:	Verifying Analyses of Manufacturing Processes Using Predictive Models and Ontologies		

Abstract:
The accuracy of predictive models of manufacturing processes has a profound impact on the efficiency and success of manufacturing processes themselves. Predictive models of manufacturing operations can be used directly and in optimizations to determine optimal process parameters to generate profits and products that meet quality standards. A faulty process of formulating these models, therefore, can significantly impede manufacturing, and technologies associated with smart manufacturing and open computing platforms have the potential to reduce these errors. This project hopes to contribute to the development of a more reliable modeling process. Specifically, the work provides a means to characterize predictive model equations by interpreting variables used in the equation's definition. To develop a methodology for evaluating these predictive model equations, the critical aspects of the model had to be isolated, analyzed, and checked for consistency. In the scope of the present work, analyzed elements are limited to proportionality between variables, desirability of effects, dimensionality, and fitness of the experimental process. The equations and their variables (recorded in IPython notebooks) were parsed into Turtle triples, then mined using the SPARQL Protocol and RDF Query Language (SPARQL). These triples were combined with a general manufacturing ontology, which categorized and assigned properties to classes and individuals representing concepts in manufacturing. This information was used in conjunction with the Apache Jena framework and the NASA Quantities, Units, Dimensions, and Types (QUDT) ontologies to analyze the accuracy of the predictive models. Relationships regarding units of measure, proportionality, and desirability of each variable were included into the general manufacturing ontology and this information was used to check for inconsistencies in the notebook data. Bayesian reasoning was applied to the ontology to determine the probability of various outcomes and the source of inconsistencies in the predictive model. The work will serve to verify some aspects of predictive models by checking that variables are treated in a manner consistent with the established ontology.

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Name: Matthew Parsons		**Grant Number**	70NANB16H101
Academic Institution: Purdue University		**Major:** Materials Engineering	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Graduate School - PhD		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Inorganic Materials Group		
NIST Research Advisor:	Dr. Chiara Ferraris		
Title of Talk:	Quantitative Analysis of Cement Paste Performance via Oscillatory Rheology		

Abstract:
Rheology, or the study of the viscoelastic properties of materials, can provide a quantitative basis on which cement past flow performance can be determined. Current rotational shear rheometry of cement paste requires large and expensive devices that use complex flow geometries, making analysis difficult, especially at the construction site. Rheological properties of cement paste are essential in application such as 3D printing or to determine the proper dosage of chemical admixture for instance.

NIST is developing a new disposable inexpensive oscillatory rheometer for cement paste. As oscillatory rheometry is not commonly used for cement paste, new testing and interpretation methods needed to be developed.

Therefore, oscillatory measurements have been compared to standard simple shear rheology data to create a framework by which the new tests can be compared to properties previously determined by simple shear, such as yield stress and initial set time. A series of oscillation tests using a standard rheometer were performed on a cement-like suspension to identify promising test procedures. The procedures were applied to cement paste for 3D printing applications.

Analysis of oscillatory rheology measurements were found to have correlations to useful quantitative measurements in simple shear rheology. The initial set time of several pastes, as determined using simple shear rheometry, was found to be similar to set times determined through oscillatory rheometry, among other correlations. These results indicate that oscillatory rheology can be used to predict the performance of cement paste, allowing for further studies on predicting the properties of cements, especially in applications such as pumping and 3-D printing.

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Name: Nathan Peterman		**Grant Number**	70NANB16H101
Academic Institution: Purdue University		**Major:** Electrical Engineering	
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	After completing four rotations of work at NASA JSC and finishing my undergraduate degree, I plan on getting a Masters in Robotics from Carnegie Mellon University		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Life Cycle Engineering Group		
NIST Research Advisor:	Paul Witherell		
Title of Talk:	Creating Design Allowables for Additively Manufactured Parts		

Abstract:
The adoption of additive manufacturing (AM) by industry has been held back due to a lack of design allowables. A design allowable provides material-process-structure relationships that result in statistically determined minimum values of a material property. Design allowables enable engineers to design parts assuming that the material will meet certain criteria, such as having a particular ultimate tensile strength. Design allowables have existed for parts made using conventional techniques, such as forging or milling, since the 1940's. However due to the large amount of process parameters that affect the properties of the finished AM part, large amounts of material properties, machine parameters, build parameters, and test outcomes need to be captured and analyzed in order to produce reliable design allowables. The Materials Data Curation System (MDCS) is a way of collecting and organizing AM material, machine, and build data into a database based on an XML (eXtensible Markup Language) schema. The schema was reviewed and annotated to gather basic information on process parameters and their relationships. Members of industry were contacted in order to gather insight on the necessary steps for developing design allowables for additive manufacturing. The material, machine, and process parameters were analyzed for importance and consolidated into a few key groups. These parameter groups act as process specifications in AM design allowables and can be varied over a predefined range in order to allow some control when producing AM parts. A literature review was conducted, and an ontology showing the relationship of the physics behind powder bed fusion was analyzed. It is expected that by grouping process parameters, minimum data requirements to characterize AM material properties can be substantially decreased. Once the relationship among the parameters has been finalized, the next step is to collect enough data to verify a normal distribution in MDCS. From a normal distribution, A-Basis (first percentile) and B-Basis (tenth percentile) design allowable values can be calculated.

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Name: Kirill Rebrov		**Grant Number**	70NANB16H093
Academic Institution: University of Texas at Austin		**Major:** BS Aerospace Engineering	
Academic Standing (Sept. '16):	Graduate student; entering UT Austin EM Graduate Program with specialization in Computational Mechanics for Fall 2016 semester		
Future Plans (School/Career):	MSE/PhD in Computational Mechanics		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Engineered Fire Safety Group		
NIST Research Advisors:	Dr Marcos Vanella and Dr Randall McDermott		
Title of Talk:	A correction for velocity penetration error at immersed boundaries in the Fire Dynamics Simulator (FDS)		

Abstract:
This effort involves development of a 3D test problem code in an attempt to improve the accuracy and efficiency of the NIST Fire Dynamics Simulator (FDS) software. FDS is an open source, computational fluid dynamics package which models fire propagation; it outputs the numerical solution to the system of partial differential equations governing fluid flow. Manipulation of the momentum governing equation results in the pressure Poisson boundary value problem – a region of interest is characterized by the governing differential equation, with values prescribed along its external boundaries. Hence, a solution to this differential equation must satisfy its boundary conditions on the domain. This classic boundary-value problem may be further developed by means of introducing an immersed obstacle into the domain; this creates a submerged solid region within the fluid domain extension, necessitating internal boundary conditions at the obstacle-domain interface. Information on the computational domain is stored through a uniform grid definition with staggered arrangement – the problem region is discretized into square cells of equivalent size, with scalar variables stored at the center of these control volumes, and velocity variables at cell interfaces. In theory, velocity penetration at immersed boundaries should be zero (there should be no fluid flow between immersed obstacles and problem domain); however, the computational pressure field currently generates a penetration error, whereby nonzero velocities "bleed" through immersed boundaries. A pressure correction field must be added to compensate for velocity penetration error; this projection scheme also ensures the solution's compliance with the thermodynamic divergence of the system. Multiple Poisson solver routines are investigated to assess respective efficiency savings.

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Name: Patrick Seiler		**Grant Number**	70NANB16H129
Academic Institution: Texas A&M University System		**Major:** Industrial Engineering	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	I plan to pursue graduate studies, but I am unsure as to specifically what I would like to study in graduate school.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Networked Control Systems Group		
NIST Research Advisor:	Timothy A. Zimmerman		
Title of Talk:	Assessing the Impact of Cybersecurity on Networked Control Systems		

Abstract:
Modern life depends heavily on Industrial Control Systems (ICS) to control numerous industrial processes such as electricity generation and distribution, food production, or manufacturing. Many deployed ICS were designed prior to the heavy reliance on networking and the Internet for ICS communications. Unfortunately, the increasing necessity to network and connect ICS has opened up new avenues for cyberattack on both legacy and modern ICS. Despite this increased danger, industry lacks extensive research and guidance on the performance impact imparted on the ICS by hardware and software designed to protect them. The NIST Networked Control Systems group set out to examine the impact of cybersecurity on ICS by measuring the overall behavior of a properly protected system. To gain a preliminary understanding of the effects cybersecurity could have on system operations, various forms of packet disturbance were introduced onto an ICS network. The types of packet disturbances utilized accurately represented performance impacts that could arise in a network protected by various cybersecurity hardware and software. The measurements initially performed on the Robotic Enclave of the ICS Cybersecurity Testbed were used to develop a baseline for modeling the reaction of a typical ICS to heightened cybersecurity measures. This baseline was then used as a point of reference for the later experiments measuring the ICS reaction to packet disturbances. Said experiments led to an accurate understanding of likely ICS reactions to cybersecurity.

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Name: Tawsif Siddiqui		**Grant Number**	70NANB16H131
Academic Institution: University of Maryland, College Park		**Major:** Computer Engineering	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Graduate school		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Information Modeling & Testing Group		
NIST Research Advisor:	Yan Lu		
Title of Talk:	Schema and Ontology Development for The Additive Manufacturing (AM) Database		

Abstract:
To promote additive manufacturing (AM) technology adoption in real production, sufficient understanding of AM geometry-material-process–structure-property relationships is required. Currently, an open Additive Manufacturing Materials Database (AMMD) is under development at National Institute of Standards and Technology (NIST) in order to collect and publish data for AM community to identify material process-structure-property relationships. This database is built using the NIST Material Data Curation System (MDCS) as a backend with structure provided by NIST's AM schema. In this project, first I helped the project team to enhance the data schema. annotate the data schema and populate the database with the data from NIST AM tests. A preliminary draft of the schema annotations has been created, which makes the schema more understandable for the general users. With a web based tool provided by MDCS, NIST AM test data are captured in the Am material database. Another important part of my involvement in the project is to create an ontology for the AM database navigation. A well designed AM data navigation pane is very important for user to explore and search data. Furthermore, as an open database, both the AM navigation schema and data schema could be modified in the future. Hence NIST AM database system is designed to allow future changes. The flexibility of the navigation comes from an ontology based configuration tool. The ontology is being developed using Protégé, where AM data navigation schema is defined by the class hierarchy and the data query is provided by the annotation. My contribution in the AM database navigation ontology development plays critical role in the first release of the NIST AM material database. The openly accessible database is set to evolve through sharing of the AM schema and pedigreed material data among the stakeholders in the AM community.

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Name: Adam Springer		**Grant Number**	70NANB16H087
Academic Institution: Northern Illinois University		**Major:** Mechanical Engineering	
Academic Standing (Sept. '16):	1st year Graduate School		
Future Plans (School/Career):	Master's of Science in Mechanical Engineering at Northern Illinois University		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Production Systems Group		
NIST Research Advisor:	Justin Whiting		
Title of Talk:	Dynamic Characteristics of the Recoater Arm used in the Direct Metal Laser Sintering Process		

Abstract:
Additive Manufacturing, dubbed 3D printing by the media, is making large advancements in the manufacturing world. This push for additive manufacturing is because of additive manufacturing's ability to quickly and easily produce complex geometries. One of the biggest problems preventing additive manufacturing from replacing traditional, subtractive methods is the lack of repeatability. It can be very difficult to reliably replicate a part with the same properties. Having accurate models that can show what is occurring during the building process would be a big step forward to gaining the consistency that is needed. Researchers are currently creating DEM (Discrete Element Method) models of the powder spreading present in the DMLS (direct metal laser sintering) process. The damping and stiffness characteristics of the recoater arm would help substantially in creating these DEM models. The ability to visualize and understand how powder is spread and how this spreading is affected by vibrations and deflections in the recoater arm are essential to controlling the process. The research being conducted will use a dynamometer and dial indicator to measure the deflections of the recoater arm as a function of the applied load along the length of the arm. These measured deflections and loads will be used to calculate the stiffness of the recoater arm as a function of location. Also, multiple accelerometers and an impact hammer will also be used to perform modal analysis which will result in the natural frequency and damping of the recoater arm. The stiffness and damping, along with other characteristics acquired from the data, will be used to model the spreading of powder in the DMLS process. These models will help in understanding and eventually controlling the process.

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Name: Alexander Stoddard		**Grant Number**	70NANB16H078
Academic Institution: Davidson College		**Major:** Mathematics, minor in Experimental Physics	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	I aspire to pursue a career either in engineering industry or in math education. I am passionate about the STEM fields and hope to make useful my knowledge and skills in them.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems, Production Systems		
NIST Research Advisor:	Gregory Vogl		
Title of Talk:	Squareness - Numerical Errors in The Utilization of Machine Tools for Engineering Processes		

Abstract:
When a production facility uses a machine tool, such as a mill or lathe, to manufacture a new product, seemingly negligible errors in the positional accuracy of the tool can severely damage the integrity and precision of the produced part. An error of a few micro-meters (an extremely short length) or micro-radians (an extremely acute angle), if not properly considered and adjusted for, can detrimentally impact the manufacturing process, causing the part to fail expected specifications or criteria. Squareness refers to the variations in the angle between two axes that are oriented to form a 90-degree angle between them. This can be measured through the use of an experimental setup that involves a ball-bar; then, the squareness can be compensated within the machine controller. However, squareness errors change with time, and ball-bar tests are not typically used with regular frequency to track these errors that impact part quality.

In an attempt to measure squareness errors very quickly with minimal experimental setup, manufacturers could potentially use accelerometers to measure the squareness along the x-, y-, and z- axes of the machine tool. These accelerometers can be attached to the machine tool to track its position during testing. However, such sensors unavoidably produce noise, which can itself impact the precision and accuracy of this method. We performed numerical simulations to determine the impact of noise on the precision of this proposed method. Specifically, the squareness is included in a set of nonlinear kinematic equations that model the collected data. Newton's method was used to solve these nonlinear equations from a least-squares approach. Finally, the relationship between the squareness and the noise level was determined based on these simulations.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Vaughn Varma		**Grant Number**	70NANB16H091
Academic Institution: Rochester Institute of Technology		**Major:** Mechanical Engineering	
Academic Standing (Sept. '16):	Graduate Student at RIT		
Future Plans (School/Career):	MS in Mechanical Engineering, MS in Computer Science, Robotics R&D (Automation, Synthetic Intelligence), Battlebots		
NIST Laboratory, Division, and Group:	Engineering Lab, Systems Integration Division, Information Modeling and Testing		
NIST Research Advisor:	Yan Lu		
Title of Talk:	The Internet of Things on the Shop Floor: Design and Implementation of a Service-Oriented Architecture in Manufacturing Systems utilizing B-SCADA's Status Enterprise		

Abstract:
The goal of this project is to implement a Service-Oriented Architecture (SOA) system on a manufacturing shop floor; such a system has the potential to provide substantial benefits to production lines, improving versatility, flexibility, and robustness. This investigation is specifically to explore the capabilities of Status Enterprise, an Open Platform Communication – Unified Architecture (OPC-UA) compliant data modeling and industrial automation software made by B-SCADA, in the context of implementing a distributed network of manufacturing machines which communicate with one another to accomplish a common goal (SOA). Similar systems have been implemented at a test-scale, using various other software, and the objective of this investigation was to implement a similar system using a software with a stronger rapport in industry, Status Enterprise. Two major issues arose, such as the challenge of handling multiple concurrent client requests, and the challenge of automatic device registration. To test solutions to these issues, a mock-up use case was developed. In the end, it was discovered that Status Enterprise serves as a suitable software suite for the purposes of this project. This consequently warrants further investigation into the synthesis of an SOA system based on Status Enterprise.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Katrina Wakeman		**Grant Number**	70NANB16H097
Academic Institution: American University		**Major:** Public Health	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	After graduating, I plan on working for a few years before continuing on to get a graduate degree.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Wildland Urban Interface Fire Group		
NIST Research Advisor:	Erica Kuligowski		
Title of Talk:	Alerting the Public in Community-wide Disasters: A Literature Review on Outdoor Warning Sirens		

Abstract:
In May 2011, Joplin, Missouri was hit by an EF-5 tornado which caused 161 fatalities and more than 1,000 injuries, making it the deadliest single tornado on record since official record-keeping began in 1950. NIST completed a technical investigation of the tornado, and recommended that national codes, standards, and guidance be created for tornado alerts and warnings. Alerts are used to grab the public's attention, while warnings are meant to provide information about the incoming hazard. In tornado prone areas, outdoor warning sirens are one of the most heavily relied upon alerting systems. However, there is almost no standardization with regards to the use of these systems. While guidance does currently exist on siren usage, many lack specifics and/or documentation of the basis upon which the guidance was developed.

The purpose of my project was to gain a comprehensive understanding of the available research regarding how people respond to alerting systems (in general), to eventually inform a set of standards and guidance for tornado outdoor warning sirens. Studies from multiple disciplines, including acoustics, crisis management, human factors, sociology, and education were reviewed and synthesized. The findings from these various disciplines allow for conclusions to be drawn regarding best practices on the use of siren systems.

Overall, this literature review answered many questions, including which sounds are best at grabbing the attention of the public, which sounds evoke perceived urgency, whether or not information needs to be provided with the sirens, how often sirens should be sounded, which demographics are more vulnerable to tornadoes, what methods are available to educate a community about disaster protocol, and what are the benefits of standardization. This literature review will be used to inform a guidance document for tornado-prone communities on the creation and provision of public alerts via outdoor siren systems in tornado emergencies.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Samantha Weaver		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland College Park	**Major:**	Chemical Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Career in alternative energy		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Polymeric Materials Group		
NIST Research Advisor:	Dr. Xiaohong Gu		
Title of Talk:	Impacts of temperature, relative humidity, and UV source on EVA degradation in accelerated weathering tests		

Abstract:
Photovoltaic (PV) products have experienced great growth in recent years; however, to become a staple of the energy infrastructure, PV products must prove their long-term durability. Solar panels, in particular, are complex and rely heavily on polymers as encapsulants, back sheets, and edge sealants. Ethylene Vinyl Acetate (EVA) is the most commonly used encapsulant, but it does experience severe degradation due to environmental conditions. This weathering stressors compromise the solar panel and can lead to module failure. Despite the environmental aging studies conducted, the mechanism of EVA's photodegradation is still not well understood, and there is no standard aging test to determine the field viability of EVA formulations.

Working with NREL and multiple industry partners, three different EVA formulations were aged and examined. This work sought to better understand the photodegradation mechanism of EVA and how it is effected by temperature, relative humidity, and ultraviolet (UV) light source. Using UV-Visible spectroscopy, FT-IR, and other tests the EVA's chemical and mechanical properties were characterized and compared. The intent was to find the driving factors of degradation, which could then, ultimately, contribute to determining the optimal accelerated weathering test.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: Shawn White		**Grant Number**	70NANB16H079
Academic Institution: Arizona State University		**Major:** Mechanical Engineering	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Planning to pursue my masters in mechanical engineering at Arizona State University		
NIST Laboratory, Division, and Group:	Engineering Laboratory (EL), Intelligent Systems Group, Production Systems Group		
NIST Research Advisor:	Brandon Lane		
Title of Talk:	Dynamic and Mechanical Properties of Metal Powder		

Abstract:
While there are many ways to investigate the properties of different metal powder particles, the most standard way is to use a funnel system called a hall flowmeter. This project focuses on using a high speed camera in an experimental apparatus with a hall flowmeter to observe gravity-fed powder flow and its collisions with a horizontal observation plate. Using this set up to record the powder flow one can use image analysis algorithms to calculate and measure the powders flow velocity, coefficient of restitution (COR) for bouncing particles, Rayleigh flow instabilities, angles of repose, and shear collapsing on the powder pile. The collected data can be used as quality metrics for the powder or provided to collaborators to calibrate their multi-physics simulations of the powder flow for discrete element modeling.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Thomas Winnard		**Grant Number**	70NANB16H098
Academic Institution: Andrews University		**Major:** Mechanical Engineering	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	A career in either the automotive or the defense industry, possibly after graduate school.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Production Systems Group		
NIST Research Advisor:	Gregory W. Vogl		
Title of Talk:	CNC Linear Axis Diagnostics via Sensors		

Abstract:
Cost reduction and time-loss minimization are fundamental operational goals of manufacturing. This is no less true in the machining industry, which relies on machine tools to fabricate parts for a diverse range of markets. Acceptable conditions of a machine tool's linear axes are central to the production of well-made parts. Current practices to measure the geometric performance of linear axes halt production on a machine tool for great lengths of time, which lead to lost revenue. Manufacturers desire quick checks for axes health that require less than 15 minutes, instead of hours or even days. This project aims to reduce the diagnosis time by measuring changes in linear axis errors via the use of sensors in a small inertial measurement unit (IMU). The sensors being used are a triaxial accelerometer and a triaxial rate gyroscope.

We first set up the IMU on a linear axis testbed and then tested our setup on a CNC (computer numerical control) machine tool. The IMU utilizes highly sensitive sensors to sense translational and rotational motions due to micrometer-level (μm-level) or microradian-level (μrad-level) linear axis error motions. Previous work on a linear axis testbed at NIST showed that the IMU-based method could be successfully applied on a machine tool. Therefore, the LabVIEW code was modified for application of the method on machine tools in NIST Shops. The two major challenges of this project were to make data collection dependent on IMU motion, rather than linear position data via the motor controller, and to set up the LabVIEW code so it could seamlessly transition between use on either the testbed or the machine tool. After fixtures were designed and fabricated for application of the IMU on machine tools, data was collected for single-axis motion on a machine tool in NIST Shops. These experiments showed that the IMU and associated data instrumentation and software are applicable for machine-to-machine usage in a manufacturing production environment.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Malachi Yeh		**Grant Number**	70NANB16H159
Academic Institution: University of Maryland, Baltimore County		**Major:** Computer Engineering	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Pursuing a PhD		
NIST Laboratory, Division, and Group:	Engineering Laboratory (EL), Applied Economics Office		
NIST Research Advisor:	Eric O'Rear		
Title of Talk:	BIRDS: Quantifying Sustainability in Commercial Buildings		

Abstract:
The Building Industry Reporting and Design for Sustainability (BIRDS) combines whole building energy simulations with life-cycling cost and life-cycle environmental assessment to develop an extensive building performance database. The BIRDS database includes cost, energy, and environmental measurements for 16 commercial building types in 229 cities across the United States. Each building can be compared over four building standard editions, location, and investor time horizon to determine the effect of energy efficiency on sustainability performance.

My work on the BIRDS Commercial database was threefold. First, extract data from whole building energy simulation results files containing information on the various building types over the four standards editions. Second, calculate the initial construction costs, annual operating energy costs, future maintenance, repairs, and replacement cost, and residual value of each building design over a 40-year study period to determine the total costs of a building over the investor's time horizon. Third, calculate the environmental impacts associated with constructing, operating, and maintaining each building.

This database will be incorporated into the BIRDS software to allow the comparison of different types of commercial building designs and how that would impact their cost, environmental impacts, and energy efficiency. Engineers and architects can use this database when designing a building while policymakers can use it to make better building standards.

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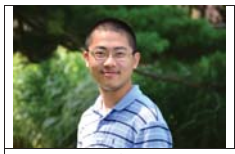
Name: Raef Youssef		**Grant Number**	70NANB16H159
Academic Institution: University of Maryland, Baltimore County		**Major:** Computer Engineering	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Engineering Laboratory, System Integration Division, Life Cycle Engineering Group		
NIST Research Advisor:	Dr. Guodong Shao		
Title of Talk:	Implementing the ISO 15746 Standard and the Optimization Metamodel for Process Parameter Optimization		

Abstract:
In smart manufacturing systems, making and planning control decisions often involves solving optimization problems. Currently, applications that implement controls are provided by vendors that are mostly independent of each other. As a result, these tools often employ different and specialized data representations. This is inefficient because data that are used by multiple tools would need to be modeled multiple times. Furthermore, it is very difficult to integrate process controls with optimization at different levels. Such integration is important because otherwise it requires a great deal of experience from factory operators to manually set and monitor process parameters.

We introduce a methodology that implements the ISO 15746 standard and a NIST developed Optimization Programming Language (OPL) metamodel for integrating advanced process control and optimization (APC-O). This SURF project focuses on automating the implementation for a manufacturing case. To describe the manufacturing process, an XML (EXtensible Markup Language) schema that corresponds to the information model specified by the standard is used. Once an XML representation of the case is obtained, it is then parsed for relevant information to the optimization problem. The information is used as input to the OPL metamodel to create an executable optimization model in OPL format. The generated OPL code is solved by a commercial numerical optimizer. The results are then used as actionable recommendation to set the corresponding process parameters.

In this project, an additive manufacturing, laser sintering process, was selected as the case study. The case study showcases the flexibility, traceability, and reusability of the methodology to automate the integration of APC-O.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Tony Zhang		**Grant Number**	70NANB16H131
Academic Institution: University of Maryland, College Park		**Major:** Electrical Engineering	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Graduate School in Electrical Engineering		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Cognition & Collaboration Systems Group		
NIST Research Advisor:	Jeremy Marvel		
Title of Talk:	Onboard Location Tracking for Collaborative Robot Applications		

Abstract:
As automation technology becomes more commonplace in manufacturing, the need for advanced, integrated monitoring equipment and algorithms becomes increasingly vital. Through improvements made to external and onboard tracking system (e.g., motion sensors and cameras), a workspace may be protected without requiring safety fences, barriers, or other physical safeguards. In the field of robotics, it is crucial to know the location of both the human workforce and the robotic equipment to ensure a safe working environment. This project investigates the performance of networked, small-scale tracking sensors that will be integrated into parts and equipment for localization and environment observation. Integrating tracking capabilities into equipment is expected to reduce localization uncertainty, as it is not subject to occlusion or environmental influences such as temperature or changes in lighting. Moreover, such tracking abilities would promote workforce safety and security and increase productivity of both people and robots in warehouse, manufacturing, and construction facilities.

This project developed and evaluated an embedded small-scale sensor suite that can be integrated into robotic configurations and wearable technologies to facilitate human-robot interactions. The sensor suite is responsible for reporting three-dimensional positions and rotations within the Collaborative Robotics Laboratory. Small, robot-mounted platforms consisting of microcontrollers obtain raw data from inertial measurement units (IMUs), light monitors, and distance sensors. Individual platforms are networked via wireless technologies, and sensor data is transmitted to a host computer that maintains a model of the world as measured by the sensors. The raw data being fed into the world model is noisy, so probabilistic noise models are used to compensate for measurement uncertainty. Filtered pose information is then transmitted to an Android tablet held by a human operator. Performance of the tracking system prototype was verified using an evaluative suite of test methods using industrial, collaborative robots through a motion capture system.

ITL/ CTL

Information Technology Laboratory (ITL) & Center for Technology Laboratory (CTL)

Addo, Derrick

Aliakbar, Soheil

Collazo-Martis, Ramon

Cooper, Samuel

Dare, Christopher

Dash, Aditya

Davila, Ian

de la Vega, Jose

Deng, Myra

Dougherty, Eric

Dunkers, Dan

Fulton, Kelsey

Henrich, Janelle

Hockley, Stephen

Indictor, David

James, Bruce

Kasner, Jillian

Lamp, Curtis

Laurenceau, Harry

Massey, Joshua

Mayer, Justin

McGovern, Emily

McHugh, Sean

Murphy, Joie

Pan, Jane

Patel, Ankur

Ratliff, Zachary

Reed III, Carroll

Rodriguez, Jr., Jose

Rogers, James

Smith, Ryan

Smith, Steven

Sriram, Vinay

Strange, Sean

Sutton, Kyle

Tilva, Rohan

Vargas, Daniel

Wilkes, Matthew

Xiong, Xinyu

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Derrick Addo		**Grant Number**	70NANB16H151
Academic Institution:	Bowie State University	**Major:**	Computer Science
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	I had the opportunity to meet people who were working with machine learning algorithms to solve problems and I thought it was interesting. I would like to find a career where I can combine machine learning with precision time synchronization		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Software and Systems Division, Information Systems Group		
NIST Research Advisor:	Derek Juba, Ya-Shian Li-baboud		
Title of Talk:	Synchronizing Video Playback on a Tiled Display Wall		

Abstract:
Video walls are, by nature illustrious and eye-catching. Applications of video walls include mobile dashboards or presentations (e.g. for disaster resilience/emergency response – staging areas for large scale disasters). In airports, flight times and status reports become easier to spot and read when spaced out over multiple monitors. Video walls aid in displaying data because it is able to show large amounts of information. The project strives to develop low-cost, flexible approach in synchronizing a video display wall. However, it is difficult for separate video players on separate machines to operate at the exact same frame rate. You can use a single centralized server to drive the display but if the network is slow it might cause the displays to go out of sync. Another way to solve this problem is to have the videos play at a specific time on each system. But with this method, the display may still go out of sync since the timing on each system is not synchronized. The overview of this research is to propose methods to solve the issue with video playback synchronization. My research investigates methods such as synchronization using the network time protocol (NTP) and the Scalable Amplified Group Software (SAGE2).

The NTP is a protocol that is used to synchronize computer clocks in a network of computers. NTP uses a symmetric architecture in which a distributed subnet of time servers operating in a self-organizing, hierarchical configuration that synchronizes clocks within the Local Area Network and to national time standards such as an ensemble of calibrated atomic clocks providing UTC (NIST) via radio, wire, or GPS. For synchronizing a cluster of nodes over a network, all nodes in the cluster must have their clocks synchronized, even when the cluster is isolated from the internet and global time sync servers. To accomplish this, the NTP daemon is installed on each Ubuntu/Linux node and configured; one node will act as the main time server, while the other nodes act as clients to the main time server.

In order to setup the display for video synchronization, we used SAGE2. SAGE2 is a cluster-based HTML viewer used for displaying elements across multiple screens. The SAGE2 browser software, based on Nodejs, uses web sockets for synchronization and data sharing between clients. Unfortunately, videos and WebGL-based applications did not work in SAGE2. Since this research is based on streaming videos for testing, we used the vlc player as an alternative. In this method, the *cron* utility software or *at* command is used to schedule a video playback at a particular time, where time is already synchronized by means of NTP.

SURF Student Colloquium
NIST – Gaithersburg, MD
August 2-4, 2016

Name: Sonny Aliakbar		**Grant Number**	70NANB16H095
Academic Institution:	Towson University	**Major:**	Computer Information Systems
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Apply to a pathways program at NIST and attend a graduate school		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Information Access Division, Visualization and Usability Group and Image Group		
NIST Research Advisor:	Mary Frances Theofanos and John M. Libert		
Title of Talk:	Can't Touch This: Usability of Contactless Fingerprint Acquisition Devices		

Abstract: Biometric authentication has become a vital part of ensuring U.S. national security. Traditional biometric devices used today include contact-based fingerprint acquisition devices. However, there are several risks linked with these systems which include the transmission of pathogens by the contact surface and the lengthy process of the biometric collection. To address these issues, industry has begun research to capture fingerprints without physical contact. Some challenges associated with this new technology are related to the usability factors as well as the accuracy and reliability when compared to the traditional devices used today. Prior to these contactless devices being adopted as the new norm for biometric authentication, there must be numerous forms of testing done which include: accuracy, reliability, repeatability, and usability. This study focused on usability, specifically the efficiency, effectiveness, and user satisfaction of three different contactless fingerprint acquisition devices. The purpose of this project is to study whether individuals with minimal fingerprint capture experience are able to walk up and successfully self-capture their fingerprints without assistance.
A sample size of 30 volunteers is used. To reduce possible order effects, participants are assigned to a counterbalanced order for the touchless fingerprint scanners. Each participant has a barcode scanner that he or she presents to a barcode scanner to signal they are ready to start the session capture and to record the collection time for a capture transaction. The testing takes place under three conditions: 1) the participant is asked to self-capture their prints on each of the three touchless scanners without assistance; 2) the participant watches an instructional video demonstrating how to capture their fingerprints prior to attempting to self-capture their fingerprints on each device; 3) the participants are assisted in successfully capturing their fingerprints for each of the devices. After each fingerprint capture attempt, participants answer questions about their experience with the scanner. After the three conditions are completed, participants answer a post-test questionnaire about their overall experience with the touchless fingerprint scanners. Finally, the participants have their fingerprints captured on a contact fingerprint scanner, similar to that currently used at NIST for image comparison purposes.

For this study, the measurements made are as follows: efficiency, defined as how quickly a participant can capture their fingerprints; effectiveness, defined as a low error rate referring to how many successful capture attempts are made with the satisfactory quality of all four fingers based on the number of capture attempt; and user satisfaction, defined as user preferences. Ideally, a positive combination of all three of these usability factors will influence the next generation contactless biometric authentication.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: Ramon Collazo-Martis		**Grant Number**	70NANB16H161
Academic Institution: University of Puerto Rico, Rio Piedras		**Major:** Computer Science	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Pursing a Computer Engineering Master Degree, or work in a company that lets me get a degree at the same time.		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division; Security Testing, Validation and Measurement Group		
NIST Research Advisor:	Dr. Apostol Vassilev		
Title of Talk:	Strong Key Generation on Conventional Computer Systems Enabled by a Remote Entropy Source		

Abstract:

An essential concept in the cyber world is the Cybersecurity. Especially when we want to communicate via internet and do not want anyone to intercept the message and be able to read it. This problem has been mitigated by the use of encryption methods such as the asymmetric encryption, which uses a pair of cryptographic keys to encrypt and decrypt the data being exchanged or used. In modern cryptography the secret is the cryptographic key, not the algorithm. Thus, it is very important for users of cryptography to be able to generate hard-to-guess keys and to keep them secret. However, keeping these keys secret could also be considered a challenge because, even though it is computationally infeasible, with enough time and powerful resources, a key could be guessed by clever attacks exploiting weaknesses in the generation of keys or in leaking information about them. EaaS [1] helps with the generation of strong keys by providing random data to client computers. The clients communicate with EaaS using a simple protocol utilizing asymmetric encryption.

A Trusted Platform Module (TPM) is a cryptographic co-processor that can securely store and generate encryption keys and is used mostly in commercial personal computers and client systems to authenticate the platforms. A TPM is also the ideal place to store important key material, such as the asymmetric key used to access the EaaS. Even though the TPM supports encryption algorithms that can generate good keys, it needs certain amount of entropy to make these key impossible to guess. We worked with a client that uses a TPM which assists the system to obtain entropy from EaaS and enable generation of strong keys. We implemented the client so it re-generates the key pair for accessing EaaS after each update with new random data, so that it becomes even more complex for attackers to guess and compromise it.

[1] Entropy as a Server project description page: http://csrc.nist.gov/projects/eaas/

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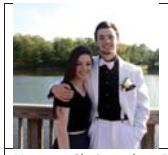
NIST – Gaithersburg, MD
August 2-4, 2016

Name: Samuel Cooper		**Grant Number**	70NANB16H083
Academic Institution: Fayetteville State University		**Major:** Computer Science	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	I am currently planning on pursuing a career in software engineering post-graduation and perhaps entering into a master's program in computer science at NC State or Georgia Tech.		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division, Secure Systems and Applications Group		
NIST Research Advisor:	Dr. Michaela Iorga, Dr. Dmitry Cousin		
Title of Talk:	Detecting malicious users and compromised accounts using user behavioral models for the C-Force Enterprise's cloud service		

Abstract:
Cloud computing is the new paradigm that rapidly evolved in the past years to offer a utility-based model for enabling convenient, on-demand network access, from anywhere, to a shared pool of configurable computing resources. Business are more and more taking advantage of this new technology by building scalable, cost-effective solutions cloud-based services.
Our C-Force Enterprise designed and securely implemented the Minecraft video game that allows our users to build structures out of textured cubes in a 3D world, to explore, gather resource, interact and communicate in a multiplayer environment that shares the single world. To secure the service we offer – the Minecraft video game - we selected an Infrastructure as a Service (IaaS) VMWare cloud where we implemented secured logging, insider threat continuous monitoring system, user behavior analytics system, system metrics and operational monitoring system.
When applications are implemented in a cloud environment, the threat vector changes making the applications potentially more vulnerable to attacks from outside sources that penetrate inside the system by stealing credentials. Our C-Force team researched and implemented a module that monitors users' activities in the cloud environment. By monitoring users' behavior, the C-Force Enterprise in the role of a cloud service provider can verify that a user behavior does not deviate from the historically consistent behavioral patterns. All events triggered by users' actions are logged in a secure way, employing cryptographic hash chaining (implementation done by Matthew Landen and Nikita Wootten, members of our C-Force Enterprise's team). The focus of my work is to validate and analyze, in near-real time, the logged information pertaining to video game users and identify, with high probability, user's behavioral patterns that deviate from the statistically-established norm. Such deviations may identify suspicious behavior of a particular user or that the user's account is compromised. Analyzing and detecting users' behavior anomalies helps our C-Force Enterprise team identify intrusions and misuse of user credentials.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Christopher Dare		**Grant Number**	70NANB16H094
Academic Institution:	Virginia Polytech. Institute & State University	**Major:**	Computer Science, Mathematics
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	Pursuing PhD in Mathematics		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division, Cryptographic Technology Group		
NIST Research Advisor:	Lawrence Bassham		
Title of Talk:	Latency of Lightweight Cryptographic Algorithms		

Abstract:

The emerging concept of Internet of Things (IoT) allows everyday devices to have network connectivity, transmitting and receiving data via a private or public host. When sending these data packets, the raw data becomes vulnerable in its plain state, such that one could simply read the plaintext if it was acquired. Cryptographic algorithms provide a methodic way of encryption by converting the plaintext into ciphertext, which can be extremely difficult to translate without a unique key.

Typically, microcontrollers embedded in everyday objects are much smaller than the Central Processing Units (CPUs) found in a computer, or even a smart phone. Thus, with a smaller processer and significantly fewer registers, there is greater need for efficiency in both latency and memory usage when encrypting data on an 8-bit microcontroller. The latency of such algorithms is compared based on the total number of clock cycles the encryption, decryption, and key schedule undergo on a given microcontroller with a set clock frequency. Currently, the Advanced Encryption Standard (AES) is the industry standard for encryption due to the cipher's strength and relatively small hardware footprint, though the cipher was designed primarily for desktops and servers. Other ciphers, such as SIMON and SPECK, were designed specifically for hardware and software applications, respectively.

After testing 10 different block ciphers (optimized to both on-the-fly key generation and precomputed keys), the results follow closely to the Fair Evaluation of Lightweight Cryptographic Systems (FELICS) - that SPECK operates with the lowest latency and memory footprint on mid-range 8-bit microcontrollers for software applications. Though the strength of each cipher is not compared, this evaluation allows certain ciphers to be more fit for consideration in software applications.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Aditya Dash		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland, College Park	**Major:**	Computer Science
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Attend graduate school for electrical engineering. Some fields in which I am interested include signal analysis and manipulation, artificial intelligence, and wireless power transfer.		
NIST Laboratory, Division, and Group:	Information Technologies Lab, Advanced Network Technologies Division, HQ Group		
NIST Research Advisor:	Abdella Battou, Charif Mahmoudi, Lotfi Benmohamed		
Title of Talk:	Performance Monitoring and Instrumentation of Named-Data Networks		

Abstract:
As the internet grows to connect an ever-increasing amount of devices and their data, the need for a more robust information-exchange framework has developed. One promising Future Internet Architecture for this need is Named-Data Networking (NDN), which is based on information-centric networking.

In contrast to today's Internet Protocol (IP) where an end-to-end connection is established between the client and host, with NDN the client requests content from the network and the network returns it. The client does this by sending an Interest Packet to the network and receiving a Data Packet. Data Packets are signed in NDN, allowing the receiver to validate that the content is correct regardless of its source. The elimination of a direct channel between content-requester and content-provider leads to lower latency and more effective bandwidth usage.

NDN is presently in its testing phase. A deployed testbed spans the globe with nodes in several major universities and institutions including NIST. The current method of managing the network involves accessing each node through a secure shell (SSH) and running shell commands in order to view properties of the node. This approach is manual and exposes the machine hosting the node to whomever is accessing the node.

This project attempts to simplify and secure the use of the NDN testbed by creating a unified graphical user interface (GUI) that allows users of different access levels to view and make changes to nodes in the testbed. Using emerging web technologies such as HTML5, Yeoman, and Google's AngularJS, the application features a single-state display of the network topology and various data from network nodes. Updates to the NoSQL database are visible to multiple clients as changes are made in real-time.

If deployed on the NDN testbed, this application will facilitate further testing of NDN and improvements on the system.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Ian Davila Morales		**Grant Number**	70NANB16H161
Academic Institution: University of Puerto Rico		**Major:** Computer Science	
Academic Standing (Sept. '16):	Junior in Computer Science, Senior in University		
Future Plans (School/Career):	Pursuing a graduate degree in Cybersecurity		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Advanced Network Technology Division, Internet & Scalable Systems Metrology Group		
NIST Research Advisor:	Douglas Montgomery		
Title of Talk:	Test and Measurement of Software Defined Virtual Networks		

Abstract:
Software Defined Networking (SDN) moves away from traditional architectures which physically decouples the network's control plane and data plane. The control plane can now be directly controlled through software. This project entails in the development of a testbed for research in the application of software defined network technology to the domain of machine to machine networking. In particular, we researched security, robustness, and performance of emerging commercial and open source implementations for SDN controllers and switches. The Ixia Network Test System was used to benchmark the performance of the testbed. Multiple SDN controller implementations emerging from industry open source efforts were tested and measured.

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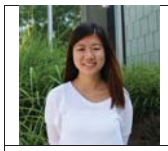
NIST – Gaithersburg, MD
August 2-4, 2016

Name: Jose de la Vega		**Grant Number**	70NANB16H161
Academic Institution: University of Puerto Rico, Río Piedras		**Major:** Computer Science	
Academic Standing (Sept. '16):	Senior (5th year)		
Future Plans (School/Career):	Get a Master's degree in Computer Engineering at the University of Puerto Rico, Mayagüez campus		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Advanced Network Technologies Division, Internet & Scalable Systems Metrology Group		
NIST Research Advisor:	Douglas Montgomery		
Title of Talk:	Test and Evaluation of Network Anomaly Detection Technologies		

Abstract:
Network-based protection systems are vital to the security of most enterprises. Some tools used to examine network behavior are the network intrusion detection (NID) and the network anomaly detection (NAD) systems. NIDs focus on searching for known attacks on the network. This is not the best way to protect your network since attackers will have the advantage because while NID developers discover, reverse engineer and develop signatures for a new attack, the attackers will already be developing another attack. NAD systems focus on monitoring the usual behavior of you network, and detecting anything that is an anomalous outlier from what is normal. This is better than searching for specific attacks since you may not yet know a new attack, but you do know your network.

While promising, commercially viable network anomaly detection systems are still under research and development. One of the challenges of their use is that they require training to learn how the network behaves, but the training data that is given to them is often very limited or contains sensitive information. The goal of this research is to generate fully synthetic network flows based on real flows so that the different NAD tools can be evaluated for their accuracy and efficiency. Also, we are evaluating the performance of these NAD and NID tools for various sets of test traffic.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Myra Deng		**Grant Number**	70NANB16H081
Academic Institution:	Columbia University in the City of New York	**Major:**	Computer Science/ Operations Research
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	Master's degree in Computer Science/ Operations Research, followed by a career in the tech industry		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied and Computational Mathematics Division, Computing and Communications Theory Group		
NIST Research Advisor:	Dr. Isabel Beichl		
Title of Talk:	A Probabilistic Method for Counting the Number of Linear Extensions in a Partially Ordered Set		

Abstract:

Optimization of scheduling and construction planning has become increasingly significant in the modern campaign for efficiency. Developing a novel method for approximating the number of linear extensions in a partially ordered set, which is synonymous with counting the number of topological sorts in a directed acyclic graph (DAG), provides a measure of the options available when comparing possible decisions.

A topological sort is defined to be a linear ordering of vertices where for all directed edges $u \rightarrow v$, vertex u comes before v. Therefore, the number of topological sorts in a DAG represents the number of valid orderings of vertices. Counting the number of topological sorts exactly has been proven to be NP-hard. Thus in this project, we use Monte Carlo methods (methods that use repeated random sampling to obtain numerical results) to estimate this measure. Specifically, we use importance sampling techniques, which are relevant because of their ability to reduce the variance of a sample. The importance function that we will use for this sampling technique sets the probability of selecting a node to be proportional to the number of descendants of that node. A recursive algorithm was implemented in C to estimate the total number of topological sorts in a given DAG. Variances with and without recursion were then compared.

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Name: Eric Dougherty		**Grant Number**	70NANB16H100
Academic Institution:	Millersville University	**Major:**	Computer Science
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Research/work in artificial intelligence		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied and Computational Mathematics Division, High Performance Computing and Visualization Group		
NIST Research Advisor:	Sandy Ressler		
Title of Talk:	Virtual Reality on the World Wide Web		

Abstract:

Rapidly growing in availability and sophistication, virtual reality technology immerses users in computer simulated space. This project entails using the Oculus Rift and a web browser to explore how virtual content can be consumed on the world wide web.

In this project we use 360 degree cameras to record and produce equirectangular video that can be displayed natively in a web browser. We utilize A-Frame, a JavaScript framework built on THREE.js that enables creation of virtual reality scenes using Hyper Text Markup Language. Using A-Frame, we also test rendering 3-dimensional COLLAborative Design Activity (COLLADA) models in the browser.

Virtual reality requires new methods of interaction that move beyond the traditional keyboard and mouse. There are a variety of controllers and motion detectors that are currently being developed. We explore some methods of interaction within the virtual content itself using gaze detection to display textual information or allow movement between video-sphere environments.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: Dan Dunkers		**Grant Number**	70NANB16H069
Academic Institution:	Drexel University	**Major:**	Electrical Engineering
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	Dual major with computer engineering		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied and Computational Mathematics Division, Immersive Visualization Laboratory		
NIST Research Advisor:	Wesley Griffin, Judith Terrill		
Title of Talk:	Using the CIE-LAB color space to improve the analysis of tests across system differences for the CAVE (Computer Assisted Virtual Environment)		

Abstract:
Virtual and augmented realities are new technologies designed to immerse the user in what they are seeing. Systems that utilize this technology are designed to incorporate the user's hand and head-movement to add to the experience. The CAVE (Computer Assisted Virtual Environment) is an augmented reality device that is being developed to visualize data in a new environment, giving the user a feeling of immersion and a level of manipulation that a normal desktop screen cannot provide. The CAVE system uses OpenGL to render 2D and 3D graphics. OpenGL does not guarantee identical output for the same input of code, especially with different hardware and drivers. This variance that can be caused by OpenGL is acceptable for rendering objects that do not need to be precise, such as objects in games and movies. On the other-hand, variance in what you are looking at from system to system may not be acceptable while visualizing data. Current tests that challenge the reproducibility of OpenGL for the CAVE were developed to evaluate test images pixel by pixel using the sRGB color space. These tests break each pixel into its respective RGB channels and evaluate the channels one by one. This method of evaluation can lead to images that look the same but do not pass the current tests because they differ in a manner which someone looking at the two images could not perceive.

In order to improve these tests, I am exploring the use of the CIE-LAB color space in an effort to give the test's success a threshold instead of being a binary pass or fail. The CIE-LAB color space is preferred over sRGB because the Euclidean distance of two points in the color space directly correlates to the difference of the two colors perceptually. By using this color-space, we can set a threshold of how different two supposedly identical color are before they look different, and also the percentage of pixels that have to be different for a test to fail. This testing method also allows for in-depth analysis of each frame, and the comparison of multiple systems against each other.

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Name: Kelsey Fulton		**Grant Number**	70NANB16H100
Academic Institution:	Millersville University	**Major:**	Computer Science and Mathematics
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Attending graduate school to pursue a PhD in cyber security		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division, Security Components and Mechanisms Group		
NIST Research Advisor:	Lee Badger, Dmitry Cousin, and David Waltermire		
Title of Talk:	Unwinding the Runtime Stack: Application Runtime Analysis for Anomaly Detection Research		

Abstract:
Intrusion detection, the runtime monitoring of a computer system with the goal of detecting malicious activity, has become increasingly important in our modern world run by computers. While anomaly detection encompasses more than software behavior monitoring and incident response, this project at NIST focuses on applying anomaly detection techniques to detect potentially malicious software runtime behavior. The model developed here at NIST for detecting anomalous software behavior involves the logging of system calls and the program counter (PC) values from where these calls were made. When behavior begins to appear too anomalous, an alarm is generated. The problem is that nearly all system calls are issued through a standard library. This presents a problem when gathering PC values, since a PC value reflects the system call location in the library and not the calling context in the program. To find the PC values of the location just prior to the library call, the runtime stack must be unwound to the call location in the actual program. The goal of this research was to create a stack unwinding application that is source code, debugging information, and program design independent. The general layout of the runtime stack on a UNIX-like system was studied by using the GNU Debugger. An application was written to unwind the runtime stack of a C program using a very basic model of system calls. The model included four system calls with easy to recognize parameters, rather than all of the system calls present in the UNIX kernel. This gave a baseline to begin writing an application that could use these system calls as a starting point for unwinding the stack. A test script was created to verify the usability of the application in a real-world setting, and the efficiency and performance of this application was compared to that of other existing stack unwinding applications used in debugging and exception handling.

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August 2-4, 2016

Name: Janelle Henrich		**Grant Number**	70NANB16H097
Academic Institution: American University		**Major:** Mathematics, Economics	
Academic Standing (Sept. '16):	Graduated with Bachelor of Science degrees in Mathematics and Economics		
Future Plans (School/Career):	Pursuing a career in applied mathematics and eventually attending graduate school		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, ITL Lab Office, Federal and Industrial Relations Office		
NIST Research Advisors:	Dr. Martin Herman, Dr. Hariharan Iyer, and Dr. Gunay Dogan		
Title of Talk:	Finding the Matching Pair: The Use of Graph Theory in Forensic Footwear Analysis		

Abstract:
Footwear marks are often the most common form of evidence present at crime scenes. However, according to a Department of Justice publication, less than 0.3 % of requests for services received and completed in 2009 by publically funded forensic crime labs were for footwear and tire impressions. Footwear is underutilized for two fundamental reasons. First, with the possible exception of a small number of cases where randomly acquired characteristics are present, this type of evidence results in weaker associations of suspects to crime scenes than DNA or fingerprints. Furthermore, there are no reliable and accurate statistical models to determine the strength of footwear evidence, making it difficult to communicate the weight of the evidence during testimony. However, a team at NIST aims to change that by creating a prototype software system that will provide a platform for practitioners to get hands-on experience with the calculation and use of Likelihood Ratios or related measures in the context of actual footwear case work. This talk focuses on just one step towards the creation of this tool, which involves the matching of shoeprint images. Graph theory can be utilized in order to find the best mapping from one shoeprint to another, and provide measures on the quality of that mapping. This can be accomplished by finding the maximal cliques in a graph where the nodes specify a mapping from a feature in the first image in the comparison to a like feature in the second. Then, the Kabsch algorithm is utilized to find the rotational matrix and translation necessary to align the two images. This provides the ability to easily match shoeprint images that have very little noise, and partial prints. Application to noisy images will be investigated in the near future.

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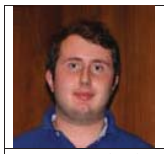
Name: Stephen Hockley		**Grant Number**	70NANB16H066
Academic Institution: Shepherd University		**Major:** Computer Science	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Pursuing a career with Intelligence Services		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Advanced Network Technologies Division, Cloud Computing Group		
NIST Research Advisor:	Dr. Michaela Iorga		
Title of Talk:	Building a Cloud Forensic Reference Architecture: Leveraging AWS CloudTrail to Identify Forensics Artifacts.		

Abstract: The Use of API Logging to Assess Forensics in the Cloud
The use of Cloud Computing by both enterprises and individuals is growing at an exponential rate. As a result, there is an increasing need to provide forensic capabilities to investigate cybercrime, cyberattacks, compliance, and related issues. Towards this end, NIST is developing a Cloud Forensic Reference Architecture to promote greater development, implementation, and use of cloud forensic capabilities. This architecture builds upon the NIST Cloud Security Reference Architecture (SRA) that leverages the comprehensive set of functional capabilities identified by the Cloud Security Alliance (CSA) in their Enterprise Architecture. Our approach in developing the Cloud Forensic Reference Architecture is to identify the functional capabilities that can potentially provide forensic artifacts. This talk focuses on how this can be done using Amazon Web Services' (AWS) CloudTrail, a framework that supports logging of API calls.

CloudTrail API logging capabilities are assessed against six AWS services that obtained provisional authorization to operate from FedRAMP, allowing AWS to offer these services to Government agencies. These services include Simple Storage Service, Redshift, Elastic Compute Cloud, Virtual Private Cloud, Elastic Block Store, and Identity and Access Management. CloudTrail logs provide specific information regarding the user's identity, request time, request action, and related information. For each of the functional capabilities, we ask: "*Does AWS CloudTrail facilitate performing forensics on the functional capability*?" If the answer is yes, then we determine, for each of the six AWS services, exactly how forensic artifacts can be obtained through the CloudTrail logs, including which *actions* in the services are relevant.



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NIST – Gaithersburg, MD
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Name: David Indictor		**Grant Number**	70NANB16H150
Academic Institution:	Binghamton University - SUNY	**Major:**	Electrical Engineering
Academic Standing (Sept. '16):	1st year Graduate Student		
Future Plans (School/Career):	Graduate school at Binghamton University, researching machine learning with Professor Kirchner		
NIST Laboratory, Division, and Group:	Communications Technology Laboratory, Wireless Networks Division		
NIST Research Advisor:	Dr. Timothy A. Hall		
Title of Talk:	Machine Learning for Spectrum Prediction		

Abstract:
The proliferation of wireless communications technologies has created wide demand for additional spectrum. Since spectrum is inherently limited, spectrum usage is governed by the Federal Communications Commission (FCC) and the National Telecommunications and Information Administration (NTIA). In order to allow for more spectrum to be available for use by non-governmental parties, a 150 MHz band of spectrum at 3.5 GHz infrequently used by the Navy has been designated for shared use as part of the Spectrum Sharing Project. Controlled by a Spectrum Access System (SAS), such a dynamic access system would grant commercial carriers the use of the band in the absence of Navy spectrum activity. In the absence of Navy and commercial carrier activity, third party users would be allowed to use the band.

Since commercial carriers have paid for use of the spectrum space, their communications must not be hindered by third party activity. Prediction of spectrum space occupancy is useful to this effect by attempting to minimize the number of instances where third parties are allowed to start transmitting but are interrupted by the SAS due to a request for higher priority transmission from commercial carriers.

Machine learning utilizes algorithms that find patterns and relationships in data and is a strong contender for many prediction problems. The problem presented here is the use of machine learning to predict whether spectrum space will be occupied by a commercial carrier. An overview of the project is presented, as is a brief overview of machine learning in the context of our prediction problem and the specific prediction algorithms we tested on our data. A comparison of the performance of the algorithms we used is also presented. The overall viability of machine learning as a means of predicting spectrum activity will be discussed.

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Name: Bruce James		**Grant Number**	70NANB16H159
Academic Institution:	University of Maryland Baltimore County	**Major:**	Mathematics
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Pursuing research in pure mathematics		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Software and Systems Division, Information Systems Group		
NIST Research Advisor:	Alden Dima		
Title of Talk:	Out of Time: Abstracting Temporal Constraints from Time-Based Data in Non-relational Databases		

Abstract:
Machine-generated sensor data are invaluable to the analysis of manufacturing processes. The data are timestamped at each sensor reading, creating a sequence of discrete events. This data may be grouped into documents when stored in a non-relational database, leading to choices in modeling and query design that may have unexpected consequences.

We investigate MIT's Alloy, a lightweight formal language-based tool modeled after the Z specification language, as a fully automated analyzer and model finder. We begin with a study of the relational structure of the core ontology of time (OOT) for the semantic web as an upper ontology on a unit manufacturing process (UMP). Alloy is then applied to model primitive types in the OOT. With the advantage of Alloy's declarative language style, we hope to exploit any polymorphism existing between the temporal logic inherent in a series of timestamp data, and the relational structure inferred from the domain-specific representation of a UMP. Our goal is to understand if lightweight-modeling tools can assist with query design and modeling of time-based data.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: Jillian Kasner		**Grant Number**	70NANB16H136
Academic Institution: Hood College		**Major:** Mathematics	
Academic Standing (Sept. '16):	Recent Graduate		
Future Plans (School/Career):	Pursue a career in statistics or cryptology		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Statistical Engineering Division, Statistical Design, Analysis, and Modeling Group		
NIST Research Advisor:	Adam Pintar		
Title of Talk:	Simulation study of an automated threshold selection for Poisson process extreme value models		

Abstract:
The design of reliable yet economic structures requires an accurate characterization of the extreme wind induced stresses they must withstand. Those stresses are deterministically related to speed, so predictions of extreme wind speeds in the field and in wind tunnels are important inputs to structural design. Recently, the Information Technology Laboratory (ITL) and the Engineering Laboratory (EL) at NIST have been collaborating to promote the use of peaks-over-threshold extreme value models over classical extreme value models. One reason for the preference is that they generally admit more data for estimation purposes, reducing uncertainty. Classic extreme value models have historically been preferred to peaks-over-threshold models by wind engineers, in part, because the latter requires the selection of an appropriate threshold. Further, the chosen threshold can have a nontrivial impact on the final predictions. Part of the ITL/EL collaboration has involved the development of a criterion on which the automatic selection of an optimal threshold can be based. My project was aimed at evaluating, through simulation, the accuracy of peaks-over-threshold model predictions that incorporate this automatic selection procedure. Since the estimation of the parameters in peaks-over-threshold models is driven by the largest observations, simulations were conducted under various distributional assumptions, loosely based on the distributional properties of real data from the field and wind tunnel. For the cases most closely resembling the real data, the results are very encouraging showing the absolute error percentage is between 5 % and 20 %, depending on the amount of extrapolation required.

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Name: Curtis Lamp		**Grant Number**	70NANB16H070
Academic Institution: Shippensburg University		**Major:** Applied Mathematics and Computer Science	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Graduate school for either applied mathematics or computational science		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Information Access Division, Visualization and Usability Group		
NIST Research Advisor:	Mary Theofanos & Haiying Guan		
Title of Talk:	Quantifying Latent Fingerprint Preprocessing		

Abstract:
Forensic latent fingerprint preprocessing covers all the image transformation activities from the latent fingerprint image directly collected from the crime scene ('before image') to the image used for identity analysis ('after image'). The preprocessing directly affects the performance of fingerprint recognition. However, this phase has received less attention, and therefore there are fewer guidelines, rule sets, or standards.

When a fingerprint markup is conducted, the latent examiner color codes portions of the fingerprint image based upon a readability scale. This process results in a fingerprint quality map. Using quality map data from the Latent Fingerprint Preprocessing Dataset, this study aims to quantify the effectiveness of image preprocessing techniques by analyzing fingerprint markup images before and after preprocessing.

The data in the Latent Fingerprint Preprocessing Dataset was collected over a three-year period and compiled into a database. Before any analysis of this data could be conducted, the database needed to be organized, cleaned and validated. Once the integrity of the database was ensured, analysis could begin. The metric used to quantify the finger print image quality given the quality map was Overall Clarity which was developed by Hicklin, Buscaglia and Roberts. This objective metric is used to compare the readability of the image before and after processing. Preliminary results suggest that lower quality latent prints can be improved by preprocessing, but sufficiently readable prints may be degraded by preprocessing.

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Name: Matthew Landen		**Grant Number**	
Academic Institution: University of Maryland, Baltimore County		**Major:** Computer Science	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Obtaining a PhD in Computer Security		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division		
NIST Research Advisor:	Michaela Iorga		
Title of Talk:	Chaining the Cloud, The C-Force's Cryptographic Hash-Chaining Logging Approach		

Abstract:

Cloud computing is the new paradigm that rapidly evolved in the past years to offer a utility-based model for enabling convenient, on-demand network access, from anywhere, to a shared pool of configurable computing resources. Businesses are taking advantage of this new technology by building scalable and cost-effective cloud-based services. Our C-Force Enterprise's team modified an open source variation of Minecraft, a video game that allows users to build structures out of textured cubes in a 3D world, to explore, gather resource, interact and communicate in a multiplayer environment that shares a single world. To secure the service – the Minecraft video game - we selected an Infrastructure as a Service (IaaS) VMWare cloud where we implemented secured logging, insider threat continuous monitoring system, user behavior analytics system, system metrics and operational monitoring system.

To ensure the integrity of the log files, the enterprise implemented Hash-Chaining, a cryptographic approach proposed by ITL's John Kelsey. This method leverages hash functions which are used to prove data integrity by applying a one-way function to data of arbitrary length and output a unique, fixed stream of bites. The chaining and validation leverages a property of hash functions which ensures that two distinct inputs will produce distinct outputs. Each logged information (or payload) is put into a chain where the hash of the previous payload is included in the current record linking the last record to all previous records. By creating logs in this manner, we can verify that there were no malicious modifications of the logs. The verification approach can be employed by a continuous monitoring module that can periodically verify the hash chain and detect, in real time, an insider threat event when any part of the log was tampered with. This logging system proves that the hash chaining approach defends against tampering of log files in cloud environments.

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Name: Harry Laurenceau		**Grant Number**	70NANB16H151
Academic Institution: Bowie State University		**Major:** Computer Science	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Upon graduating, I hope to start my career in software engineering and eventually own a technology-based start-up aimed at developing solutions to some of the world's toughest problems		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied & Computational Mathematics, High Performance Computing and Visualization Group		
NIST Research Advisor(s):	Judith E. Terrill, Terrence Griffin, Paul Patrone (Collaborating Scientist)		
Title of Talk:	Investigating the mechanics of failure through visualization		

Abstract:

Thermoset polymers are integral to the composite materials utilized in the manufacturing of advanced aircraft, such as Boeing's iconic 787. However, the mechanisms by which these materials fail are not entirely understood. Due to this deficiency in understanding, parts are often over-engineered to compensate for the uncertainty in the design, thus adding extraneous weight and bulk to aircraft. The goal of this research is to better identify the cause of the material's failure under extreme loads, thus allowing engineers to design and develop materials more efficiently without compromising safety.

There is collaboration going on between industry and NIST to try to improve the materials simulations of these polymers such that they can be used to pinpoint the cause of failure. These simulations, however, generate large quantities of numerical data and figures that, by themselves, would render data examination both useless and counter-intuitive. In an effort to ameliorate data analyzation, my team and I are using the data to create useful visualizations and visual analytic tools so that the collaborating scientists can better examine the data as well as find any flaws in the simulations, and ultimately gain better insight towards a solution.

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Name: Joshua E. Massey		**Grant Number**	70NANB16H159
Academic Institution:	University of Maryland, Baltimore County (UMBC)	**Major:**	Computer Engineering
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Advanced Network Technologies Division		
NIST Research Advisor:	Frederic J. de Vaulx and Lotfi Benmohamed		
Title of Talk:	C-Force Enterprise: Towards an Implementation of NCCP Cloud Metrics Model		

Abstract:

Cloud computing is the new paradigm that offers a utility-based model for enabling convenient, on-demand network access, from anywhere, to a shared pool of configurable computing resources. Incorporating an open-source version of the popular video game Minecraft, our C-Force Enterprise implemented secured logging, an insider threat continuous monitoring system, a user behavior analytics system, a system metrics database, and an operational monitoring system to secure Minecraft on an Infrastructure as a Service (IaaS) VMWare cloud.

Cloud-based services are typically delivered to users through various Cloud Service Providers. Although most services have similar underlying characteristics, a large challenge end-users face is comparing similar services from different providers. Additionally, metrics used to describe and measure cloud services can also vary among providers. Using the structure of a Cloud Service Metric (CSM) as defined by NIST, we standardize the way metrics are stored and how they are continuously monitored.

In the NIST-defined CSM model, a cloud service metric is broken down into four main components – the Metric itself (what is being measured) and its underlying Rules (constraints), Parameters, and an Expression. This model allows for metrics to be easily organized and stored in a manner accessible to users who wish to monitor them. For storage of our metrics, we deployed a MongoDB database, a NoSQL alternative to the traditional relational database. Our database is interacted via an application programming interface (API) which allows the user to create, read, and update stored information. A web-based graphical user interface was developed using AngularJS, a dynamic web application framework, to provide information to the API.

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Name: Justin Mayer		**Grant Number**	70NANB16H128
Academic Institution:	University of the District of Columbia	**Major:**	Computer Science
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Possible grad school, otherwise ideally some form of entrepreneurial tech innovation or a job in the tech sector.		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied & Computational Mathematics, High Performance Computing and Visualization Group		
NIST Research Advisor:	Judith E. Terrill, Terrence Griffin, Paul Patrone (Collaborating Scientist)		
Title of Talk:	Investigating the mechanics of failure through visualization		

Abstract:

Thermoset polymers are integral to the composite materials utilized in the manufacturing of advanced aircraft, such as Boeing's iconic 787. However, the mechanisms by which these materials fail are not entirely understood. Due to this deficiency in understanding, parts are often over-engineered to compensate for the uncertainty in the design, thus adding extraneous weight and bulk to aircraft. The goal is to better pinpoint what causes these materials to fail under extreme loads, and thus be able to design the aircraft using materials much more efficiently without compromising safety.

There is collaboration going on between industry and NIST to try to improve the materials simulations of these polymers such that they can be used to pinpoint the cause of failure. These simulations, however, just generate large quantities of data and are not very intuitive by themselves. We are using this data to create useful visualizations and visual analytic tools so that the collaborating scientists can better peruse the data and find the flaws in the simulations, and have better insight towards a solution.

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Name: Emily McGovern		**Grant Number**	70NANB16H159
Academic Institution:	University of Maryland Baltimore County	**Major:**	Mathematics
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	I hope to pursue a PhD in Mathematics and work in cryptography.		
NIST Laboratory, Division, and Group:	Information Technology Lab, Computer Security Division, Cryptographic Technology Group		
NIST Research Advisor:	Lily Chen, Meltem Sonmez Turan		
Title of Talk:	Analyzing the permutation testing methods of NIST SP 800-90B		

Abstract:
Random numbers are used in cryptography for many different purposes. Noise sources (e.g. radioactive decay or atmospheric noise) are used to generate these random numbers and the amount of entropy (uncertainty) produced by a noise source is very important because it determines how effective that noise source is. NIST Special Publication 800-90B outlines a method for calculating entropy for noise sources. An important part of this method is a test to see whether noise source output sequences are independent and identically distributed (IID), because this determines the track with which to test the entropy source. We will test the effectiveness of the permutation testing method described in this publication by running various tests written in Python. We tested sequences that were both known to be IID and known to be non-IID and compared the results, as well as seeing what effect sample space size and sequence length had on the results of the tests. We used both real world noise source outputs and sequences generated by the random.randrange function in Python. We noticed, among other things, that the number of distinct values generated by a particular test statistic affected the overall effectiveness of the test.

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Name: Sean McHugh		**Grant Number**	70NANB16H094
Academic Institution:	Virginia Polytech. Institute & State University	**Major:**	Computer Science
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	Graduate school for Computer Science		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Information Access Division, Image Group		
NIST Research Advisor:	Jonathon Phillips		
Title of Talk:	A Meta-Analysis on Super-Recognizers: Experts in Facial Recognition		

Abstract:

The ability of people to recognize faces exists on a broad spectrum. At one end are face blind individuals, who struggle to recognize faces of family members and friends. The other end contains individuals who possess an extraordinary ability to remember and recognize faces, referred to by the media as super-recognizers. Police employ super-recognizers as facial examiners, who pinpoint suspects from computer-generated arrays of possible matches. The most well-known use of super-recognizers is the Metropolitan Police in London, which created a super-recognizer unit that successfully identified hundreds of criminals from closed-caption television (CCTV) videos.

The first scientific paper documenting super-recognizers was published in 2009 and demonstrated their expertise. Since then, additional groups have replicated those results and studied the effectiveness of super-recognizers' implementation at practical tasks, such as forensic facial examination. The aim of my research is to summarize and analyze major works regarding super-recognizers. I compared super-recognizers' performance on facial recognition tests to control groups (representative of the general population) across various studies. In this, I discover that a person is considered a super-recognizer if they are in the 90th percentile. This corroborates that super-recognizers possess exceptional ability in facial applications. In addition, in all control groups, there are individuals with the same abilities as super-recognizers—they walk among us in the general population.

Facial forensic examiners are trained to compare face images and report their findings in court. Facial examiners have also been shown to be in the 90th percentile. Currently, it is unknown what the overlap between facial forensic examiners and super-recognizers is. It may be that facial forensic examiners were already super-recognizers and subsequently became examiners; or does training significantly improve performance? In my talk I will touch these questions and discuss future research directions.

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Name: Joie Murphy		**Grant Number**	70NANB16H068
Academic Institution:	The College of New Jersey	**Major:**	Computer Science
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Career in software engineering		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Software & Systems Division, Cyber Infrastructure Group		
NIST Research Advisor:	Spencer Breiner, Eswaran Subrahmanian, & T.N. Bhat		
Title of Talk:	Implementing distributed interfaces: tools from natural language and mathematics		

Abstract:

This project builds on previous work in which a rule and root based method was developed for generating a reusable and standardized terminology for the semantic web. The root and rule based approach is a general method for generating sets of terminologies from documents containing natural language with the goal to avoid ambiguity and normalize semantically similar phrases. In collaboration with SURF student Matthew Morse, we have developed an improved interface tool to make use of this method to increase the search power on document repositories. With the addition of semantic searching on keywords generated from both the content and metadata of a document, a user is able to query a database on more than one term and receive more significant search results. The interface, now available on the NIST INet, allows users to search on NIST Publication repositories using this approach. The web application has been constructed on a modular database system, allowing for reuse of code for similar document repositories.

In root and rule based systems, we use structured and natural language to organize queries and data in a consistent and normalized manner. For more general systems, we can extend our ability to organize information through the introduction of category theory. Category theory is a branch of mathematics that links different conceptual ideas for representing and comparing information. However, current software based on category theory has limitations which restrict the use of categorical methods in teaching, research, and engineering applications. To begin addressing this gap, we conducted a survey of individuals who use of category theory in their own disciplines (e.g., mathematicians, software engineers), asking about their past or present use of category theory software and their ideal uses of such software. Based on the requirements collected, we have begun the development of use cases and designs for future software based on category theory.

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Name: Jane Pan		**Grant Number**	70NANB16H159
Academic Institution:	University of Maryland Baltimore County	**Major:**	Mathematics & Statistics
Academic Standing (Sept. '16):	1st year graduate student at UCLA		
Future Plans (School/Career):	Pursue a PhD in Biostatistics and subsequently work on independent research at a national lab or agency.		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Statistical Engineering Division, Statistical Design, Analysis & Modeling Group		
NIST Research Advisor:	Hari Iyer Steve Lund		
Title of Talk:	Impact of Model Uncertainty on Statistical Inferences		

Abstract:

Statistical models are effective tools that can be used to estimate values of unknown quantities based on measurements which are subject to random errors. An estimate, by itself, is of little or no value unless it is accompanied by a statement of its margin of error, which is the result of sampling variability of data and choices of distributional models. Typically, the component of uncertainty arising from modeling choices is ignored, resulting in underestimation of uncertainty. A common way to measure the goodness-of-fit of a statistical model is by using a statistical test known as the Kolmogorov-Smirnov test (KS-test), which is a nonparametric statistical test for judging the plausibility of a proposed theoretical distribution as the source of the sample data. Any cumulative distribution which falls entirely within the associated Kolmogorov-Smirnov (KS) confidence band may be considered as a plausible distribution to represent observed sample data.

The main objective of my project is to develop an algorithm that can randomly generate a distribution whose cumulative distribution function (cdf) falls within the KS-band. Such distributions may be regarded as possible models for the observed data. The algorithm should also be capable of accommodating the constraint that the generated distributions are unimodal. With the help of this algorithm we are able to assess the impact of modeling assumptions on uncertainty characterizations. We will illustrate the application of this algorithm using NIST data on Standard Reference Materials (SRMs).

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Name: Ankur Patel		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland, College Park	**Major:**	Mathematics
Academic Standing (Sept. '16):	1st year Graduate Student		
Future Plans (School/Career):	Graduate School at University of North Carolina, Chapel Hill		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Statistical Engineering Division, Statistical Design, Analysis & Modeling Group		
NIST Research Advisor:	Dr. John Lu		
Title of Talk:	Evaluation of a Plenoptic Camera for Capturing 3D Footwear Impressions		

Abstract:
Latent prints from footwear and tire treads are common evidence collected during crime scene investigations. Currently, impressions are captured using 2D digital single-lens reflex (DSLR) photography, and 3D impression evidence can only be recovered either by casting and lifting. However, the physical process of casting and lifting destroys the original impression and is time-consuming and tedious to execute properly. Plenoptic cameras, which have a microlens array in front of the sensor, can provide both all focus 2D photography as well as 3D depth map which quantifies the wear pattern and allows dimensional measurements of randomly acquired characteristics such as cuts, holes, and tears in the sole of footwear. I will demonstrate the results using a high resolution Raytrix camera and associated software to capture and to reconstruct the 2D and 3D impressions from a pair of shoes which made those impressions. I will evaluate the quality of the measurement results from the Raytrix camera through existing image processing software packages to assess the presence and correlation of individual characteristics that were captured in the measured images from impressions and soles that may help define the uniqueness of a sole.

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Name: Zachary Ratliff		**Grant Number**	70NANB16H129
Academic Institution:	Texas A&M University	**Major:**	Computer Science
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	I plan to attend graduate school as well as pursue a career in either Cybersecurity or Software Engineering.		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division, Security Components & Mechanisms Group		
NIST Research Advisor:	Rick Kuhn		
Title of Talk:	Measuring the Combinatorial Coverage of Software in Real Time		

Abstract:
Combinatorial testing methods provide a cost-effective approach to achieving high assurance in mission and life critical software systems. Previous research investigating the number of factors involved in software failures showed that most failures are induced by a single factor fault or by the joint combinatorial effect of two factors, with progressively fewer failures induced by interactions between three or more factors. By testing up to 3-way or 4-way combinations of inputs and configurations, we can be reasonably confident that our system will not fail. This confidence is nearly equivalent to that of exhaustive testing when we increase our covering arrays to cover all 6-way combinations of these parameters. In many existing models however, test suites have already been generated that likely cover a significant portion of various t-way combinations. Measuring the t-way coverage of these existing test suites can allow us to determine which combinations have not yet been tested as well as determine approximately how reliable the current system is. Tools have been developed to measure this coverage but are limited to measuring static input files.

This project aimed to expand the existing, "Combinatorial Coverage Measurement Tool" to a command line version with capabilities to measure combinatorial coverage in real time. Applications of this functionality are wide ranging and include various areas of software reliability. By hooking input from live systems into the tool, organizations can determine how much of the input domain has been tested at any given time by the current users. This can be useful in determining the efficiency of testing teams and their methods, as well as deciding when a system has been thoroughly tested and is ready for launch. Another interesting area of applicability for the tool is in covering array optimization, which could be very useful in minimizing testing costs.

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Name: Carroll Reed III		**Grant Number**	70NANB16H151
Academic Institution: Bowie State University		**Major:** Computer Science	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	I plan to go on to graduate school after earning my bachelor's degree. I will stay in school until I attain a doctorate degree and plan to work within either the private sector or with the government while working towards this goal.		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Advanced Network Technologies Division, Internet and Scalable Systems Metrology Group		
NIST Research Advisor:	Scott Rose		
Title of Talk:	Scan and Analysis of HTTPS Certificates Used in the .gov Domain		

Abstract:
In recent years there has been a major surge in the number of cyberattacks perpetrated against governments, business, and personal computer networks. These attacks can result in the theft of sensitive data and incur significant cost due to fraud or network downtime. One such cyberattack is to monitor Internet traffic for private information to websites not being configured to only allow for secure connections through Secure Socket Layer/Transport Layer Security (SSL/TLS) protocols and settings. The goal of the project was to develop a tool to scan through a list of web URL's and attempt to establish a secure connection with the web server. If a secure connection was available (or the tool was redirected to a secure service), the tool obtained the X.509 certificate and certificate information associated with the web site. Once the list was processed, the collection of certificates was analyzed and statistics were compiled such as the number and names of major Certificate Authorities used, the algorithm and key length stored in the certificate as well as relevant X.509 header fields. From this data, an assessment was drawn on the state of SSL/TLS implementation within the various regions of the United States. The ratio of secure to insecure connections was found to be about even but certain regions were found to have a much higher amount of insecure websites. We plan to conduct further tests with the tool by switching our SSL/TLS algorithm to see if different connection results and vulnerabilities can be found.

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Name: Jose H. Rodriguez, Jr.		**Grant Number**	70NANB16H090
Academic Institution: Texas A&M International University		**Major:** Systems Engineering	
Academic Standing (Sept. '16):	Graduate 1st year or Graduate 1st year in the spring		
Future Plans (School/Career):	I plan to pursue a career in computer/software engineering at Texas Tech or Texas A&M University and have a career in anything technology (IT, game programming/design, or computer/software engineer or developer).		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Science Division, Cryptographic Technology Group		
NIST Research Advisor:	Kerry McKay		
Title of Talk:	Health Tests of Entropy Sources on Arduino		

Abstract:
Secure communication requires strong cryptography and unpredictable cryptographic keys. The unpredictability (entropy) comes from a random bit generator component called an entropy source. Failure of an entropy source in the field may result in predictable outputs, which can undermine security. To mitigate this, entropy sources perform health tests to alert the system in the event of entropy loss. The aim of this project is to study the effectiveness of different entropy source health tests in random bit generators. This project focuses on the health tests from Special Publication 800-90B and new predictor-based health tests, all of which aim to detect large deviations from the intended behavior of the noise source. These health tests were implemented on an Arduino board and applied to simulated entropy sources. Several performance metrics were captured, providing useful insight into the application of different methods in practice.

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Name: James Rogers		**Grant Number**	70NANB16H159
Academic Institution:	University of Maryland Baltimore County	**Major:**	Mathematics
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Attend graduate school to pursue a PhD in Mathematics or Applied Mathematics, followed by a career in mathematical research		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Software and Systems Division, Software Quality Group		
NIST Research Advisor:	Dr. Paul Black		
Title of Talk:	Injection Preservation: Testing Code with Injected Vulnerabilities for Expected Results		

Abstract:
When designing new methods for software quality analysis, we desire certainty that they are able to detect known classes of bugs. To this end, we have datasets comprised of programs with known vulnerabilities to test new methods on. One such dataset is the Intelligence Advanced Research Projects Activity (IARPA) Securely Taking On New Executable Software of Uncertain Provenance (STONESOUP), a suite of 7770 cases where industry programs written in C or Java had known vulnerabilities injected into them. These vulnerabilities are self-contained "cysts" of about one page of source code each.

One generalized method of analyzing programs like these is static analysis. This method focuses on examining source code for possible bugs without limiting the possible executions to a finite number of runtime tests, and is aided by the use of tools such as Fortify and Frama-C. These tools are examples of static analyzers that, like most, use bug-finding heuristics. As such, they catch or don't catch bugs for seemingly explained reasons.

We want to gain some assurance that injecting stand-alone code with known vulnerabilities, as with IARPA STONESOUP, is a good approach to estimate how well an analyzer does in reporting existing, real bugs. Our plan was to first run the tools on all the cysts as standalone code, to get baseline results. Second, we run the tools on all the test cases, which have the cysts injected. Third, we compare the results.

We found that running the tools on the full test cases required far more work than expected, and required at least 5 hours per test case. Thus we ran only a couple dozen examples. For these cases, we found that they yielded expected results, indicating that it is reasonable to assume that, given its cysts, IARPA STONESOUP can produce intended results.

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Name: Ryan Smith		**Grant Number**	70NANB16H150
Academic Institution:	Binghamton University, SUNY	**Major:**	Mathematics & Computer Science
Academic Standing (Sept. '16):	1st year graduate student		
Future Plans (School/Career):	Graduate school for computer science		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Software and Systems Division, Software and Systems Group		
NIST Research Advisor:	Walid Keyrouz and Derek Juba		
Title of Talk:	Accelerating k-D Trees for Nearest Neighbor Search in Walk-on-Spheres		

Abstract:
For material scientists, an important material property is electrical capacitance. NIST has developed a C++ implementation of the ZENO/Walk-on-Spheres (WoS) algorithm to compute the capacitance and other significant properties of a material at the molecular level. To compute these properties, programs stochastically solve partial differential equations by simulating random walks of particles, called walkers, following Brownian Motion (BM) and observing their collisions with the molecule. WoS utilizes an accelerated form of BM in which walkers jump to uniformly distributed points on a sphere whose radius is the walker's distance to the molecule.

The primary computational bottleneck in WoS is the Nearest Neighbor search used to determine a walker's distance to the molecule. NIST's implementation uses a spatial partitioning data structure called a k-D tree, a type of binary search tree (BST) which recursively subdivides the space of points using hyperplanes orthogonal to one coordinate axis, to accelerate search time complexity to $O(\log n)$. The current implementation requires recursively dereferencing d pointers, where $d \approx \log_2(n)$ is the height of the tree, which makes it unsuitable to run on GPUs due to the high cost of memory-fetching operations.

To alleviate the high complexity of pointer-dereferencing operations, we propose a flattened k-D tree data structure in which the branching factor (i.e., the number of subspace partitions per node) is increased to 2^w where w is an integer greater than two. Our implementation organizes $2^w - 1$ hyperplanes into each node in their own BST to drastically reduce the height of the resulting k-D tree. The flattened k-D tree demonstrates a significant reduction in pointer-dereference operations, comparable performance on CPUs to nanoflann's k-D tree implementation, and potential to experience greater performance when executed on GPUs.

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Name: Steven Smith		**Grant Number**	70NANB16H159
Academic Institution:	University of Maryland Baltimore County	**Major:**	Computer Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Pursue a career researching power efficiency in circuit design		
NIST Laboratory, Division, and Group:	Communications Technology Laboratory, Wireless Networks Division		
NIST Research Advisor:	Thao Nguyen		
Title of Talk:	Calculation of Exclusion Zones for Radar Protection in the 3.5 GHz Spectrum Band		

Abstract:
In April 2015, the Federal Communications Commission (FCC) issued a Report and Order (R&O) in FCC Docket 12-354 regarding future spectrum sharing between US Navy radar and non-radar systems in the frequency band (3550-3650) MHz (3.5 GHz band). This necessitated the development of an Environment Sensing Capability (ESC) system to monitor and protect off-shore radar receivers from harmful interference from on-shore Citizens Broadband Radio Service Device (CBSD). My task was to assist my mentor in reproducing Exclusion Zones using an approach developed in the NTIA Report TR-15-517. This framework will be used for further development and implementation of algorithms to dynamically compute Protection Zones.

Exclusion Zones are geographical areas where CBSD deployed inside the zone needs to be turned off or to vacate to another channel in the presence of the incumbent. The borders of these zones are determined by the implementation and simulation of the radar and CBSD's characteristics as well as ITM and extended Hata propagation models. Ideally, the limit of any given transmitter-to-receiver distance is found when the aggregate interference caused by CBSDs to the radar receiver is less than a certain threshold (i.e., -6 dB Interference-to-Noise ratio (I/N)).

My initial work was the implementation of two correction factors for the extended Hata propagation model. The correction factors augment the median attenuation using the details of the terrain profile between the transmitter and receiver. The correction factors detect when the terrain has unique features that the base model has difficulty accounting for, such as hills, mountains and portions of open water, etc. The factors I worked on covered the cases for when the affected terrain included isolated mountains and general slopes. After those were finished, my next assignment was to assist in acquiring and incorporating a collection of more detailed, higher resolution terrain elevation files of the continental United States' coastline for the simulation to use, allowing us even more accurate predictions of the Exclusion Zone boundaries.

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Name: Vinay Sriram		**Grant Number**	70NANB16H067
Academic Institution:	Stanford University	**Major:**	Computer Science
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Future plans include attending a reputed graduate program in computer science and/or pursuing an industry career in computer science.		
NIST Laboratory, Division, and Group:	Information Technology Lab, Applied and Computational Mathematics Division, High Performance Computing and Visualization Group		
NIST Research Advisor:	Wesley Griffin, Judith Terrill		
Title of Talk:	Sampling Techniques to achieve Color Fidelity and Anti-aliasing in the Conversion of Cubic Maps to Spherical Maps for Virtual Environments		

Abstract: One of the fundamental problems in creating 360º videos for virtual reality is the transformation of 6-sided Euclidean maps of a virtual environment into spherical maps of the same environment. Six-sided cubic maps may be thought of as the set of images that six 90º field-of-vision cameras would capture if placed at the same origin and made to face in orthogonal directions relative to each other. By contrast, a spherical map is the flattened distortion of the environment projected as a sphere around an origin camera. The canonical strategy for transforming a cubic map into a spherical map consists of populating each pixel in the output image with the color of a corresponding pixel in the input image set using ray-projection. In practice, however, this procedure is subject to aliasing effects. The current spherical mapping scheme uses a sampling filter on the input image set, which, instead of simply capturing the color of a single source pixel, averages the R, G, and B values of selected points surrounding it. While this procedure does achieve a degree of anti-aliasing, initial tests indicate that the final image has a color distortion relative to the input images. Therefore, in order achieve the anti-aliasing goal while preserving the colors represented in the input image set, we study a different class of sampling strategies. These techniques sample pixels in the output space of the transformation rather than the input space. The general methodology involves first devising a sampling-agnostic software framework that allows the selection of points to be performed independently of the mapping computations. Second, we implement an analysis platform that enables input-space visualization of a given output pixel's sampling. Using these, we implement and evaluate, among other strategies, uniform sampling and multi-correlated jittered sampling as candidates to achieve the desired conversion objectives.

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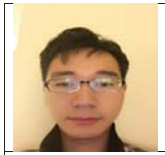
Name: Matthew Wilkes		**Grant Number**	70NANB16H084
Academic Institution: George Mason University		**Major:** Cyber Security Engineering	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Finish my undergraduate degree in Cyber Security Engineering at George Mason University followed by the pursuit of a master's degree in Cyber Security.		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Advanced Network Technologies Division, Internet & Scalable Systems Metrology Group		
NIST Research Advisor:	Yang Guo and Doug Montgomery		
Title of Talk:	Developing a Mininet Test Suite for Software Defined Internet Exchange (SDX) Research		

Abstract:

The Internet exchange point (IXP) is a network infrastructure through which different networks exchange their traffic. Software defined Internet exchange (SDX) employs a Software Defined Network (SDN) enabled switch as the IXP. At the SDX, Internet Service Providers (ISPs) can apply many diverse actions on packets based on multiple header fields, and are allowed for direct expression of more flexible policies than the conventional Border Gateway Protocol (BGP) based hop-by-hop, destination-based forwarding. SDX also enables the seamless integration of SDN networks with the conventional networks.

The goal of this project is to develop a Mininet test suite that facilitates the SDX research. Mininet is a network emulator that creates a virtual network on a single machine. It provides a simple and inexpensive network testbed for research and development. The initial phase of the project will focus on expanding the existing SDX emulator to include additional nodes and switches that are linked in various setups. The test suite will support arbitrary wide area networks with both traditional and software-defined sub-networks, and support flexible traffic forwarding policies. As a use case, the test suite will be used to study the novel BGP security technology that is made possible by SDX.



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Name: Xinyu Xiong		**Grant Number**	70NANB16H080
Academic Institution: The City College of New York		**Major:** Computer Science	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Attending Stony Brook university graduate school		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division, Secure Systems and Applications Group		
NIST Research Advisor:	Vincent Hu		
Title of Talk:	Access Control Rule Logic Circuit Simulation (ACRLCS)		

Abstract:
Access control (AC) policies can be implemented based on different AC models, which are fundamentally composed by semantically independent AC rules in expressions of privilege assignments described by attributes of subjects, actions, objects, and environment variables of the protected system. Incorrect implementations of AC policies result in faults that not only leak but also disable access of information, and faults in AC policies are difficult to detect without support of verification or automatic fault detection mechanisms.

Most research on AC model or policy verification techniques are focused on one particular model, and almost all of the research is in applied methods, which require the completed AC policies as the input for verification or test processes to generate fault reports. Those methods provide no information about the source of rule faults that might allow conflicts in privilege assignment, leakage of privileges, or conflict of interest permissions.

To address the issue, AC Rule Logic Circuit Simulation (ACRLCS) project provides an automatic method through the construction of a simulated logic circuit that simulates AC rules in AC policies -such that - - allows real-time detection of policy faults including conflicts of privilege assignments, leaks of information, and conflicts of interest assignments. For this project, I developed new critical functions (algorithms) that replace the original implementation that does not allow the inheritance capabilities nor reloading the previous saved and required to be continued work.

MML NCNR

Material Measurement Laboratory (MML)

Chemical & Biochemical Sciences

Bezio, Aaron

Bier, Imanuel

Collet, Cayla

Cross, Ebony

Filteau, Jeremy

Galvin, Connor

Hernandez, Cristopher

Jin, Emily

Knobloch, Emmie

Knowlden, Steven

Lee, Abigail

Martin, Ann Marie

McDonald, Natalie

Morse, Matthew

Patel, Nimit

Rich, Graham

Routkevitch, Denis

Rubino, Angela

Shevchuk, Mariya

Tran, Anh

Ufot, Aniekanabasi

Young, Jessica

Materials Science

Anderegg, David

Barret, Timothy

Bleakney, Matthew

Boigenzahn, Hayley

Boligitz, James

Borah, Preetom

Brandt, Samuel

Brooks, Sydney

Collini, John

Correa-Hernandez, Andres

Dasgupta, Anushka

Elquist, Aline

Gayle, Andrew

Gayvert, James

Gonzalez-Lopez, Lorelis

Hood, Sarah

Huff, Jonathan

Jeon, Heetae

Lagnese, Joseph

Lee, Erica

Locke, Michael

Luu, Norman

McCann, Gordon

Moskalenko, Andrey

Mullin, Kathleen

Nguyen, Ai

Nusinovich, Edward

Panigrahi, Atman

Peterman, Nathan

Plavchak, Christine

Schuberth, Austin

Singer, Lauren

Smith, Sarah

Stetsyuk, Karina

Stracka, Kailey

Wade, Matthew

White, Keith

Wu, Richard

NIST Center for Neutron Research (NCNR)

Ayala, Anthony

Bonk, Ryan

Fangmeyer, Ryan

Hugh, Daevin

Hunt-Isaak, Ian

Isaac, Samantha

Leos, Richard

Neves, Paul

Pasco, Madeleine

Schankler, Aaron

Scott, Douglas

Super, Nathan

Villa, Danielle

Weiss, Abdullah

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Name: Aaron Bezio		**Grant Number**	70NANB16H042
Academic Institution:	Gettysburg College	**Major:**	Chemistry
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Pursuing a career in pharmaceutical science and plan to attend pharmacy school		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Biomolecular Measurement Division, Bioprocess Measurements Group		
NIST Research Advisor:	Jeffrey Hudgens		
Title of Talk:	Development of the Next Generation of Hydrogen/Deuterium Exchange Mass Spectrometry Apparatus		

Abstract:

Hydrogen/Deuterium Exchange Mass Spectrometry (HDX-MS) is used to determine the structure of proteins, including active site identification and conformational changes. In an aqueous environment, hydrogens on amino acids will exchange with hydrogens of water molecules. While aliphatic hydrogens rarely exchange and hydrogens involved with hydrogen bonds on amino acid side chains exchange too rapidly to measure, hydrogens of backbone amides will exchange at rates that are quantifiable. The rate at which they exchange is dependent on their location within the protein as well as the type of amino acid and other nearby amino acids.

When amino acids are placed in deuterated solutions, backbone amide hydrogens will similarly exchange with deuterium in solution. When the solution is quenched, meaning the temperature is lowered and the pH is decreased to 2.5, the rate of exchange between the hydrogen and deuterium is minimized. This allows for mass analysis using mass spectrometry in order to determine which peptides exchanged for deuterium. Using this information, location of specific peptides within the protein can be determined. Typical quench conditions of 0°C and a pH of 2.5 do not slow the exchange rates enough, resulting in 25% to 30% backexchange. This means that the backbone amines continue to exchange even under quench conditions, causing less accurate mass analysis.

The objective of this project was to develop a chromatography system that could run at -30°C to further eliminate backexchange. We hypothesize that the system will lower backexchange to 6% or lower. My involvement has been with determining an ideal mobile phase A, or a solvent, or combination of solvents, that could be used so that samples cooled to -30°C would not freeze while also maintaining peak intensity of the mass spectra. Construction of the system and 3D printing of various parts have been main focuses as well.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Cayla Collett		**Grant Number**	70NANB16H163
Academic Institution:	West Virginia Wesleyan College	**Major:**	Physics/Chemistry
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Attend graduate school before pursuing a career in pharmaceutical chemical engineering		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Biomolecular Measurement Division, Bioprocess Measurements Group		
NIST Research Advisor:	Richard Cavicchi		
Title of Talk:	Protein Aggregation: Characterizing Particles Formed in Therapeutic Protein Drugs		

Abstract:

Therapeutic protein drugs are antibodies that provide a unique treatment option for many diseases and disorders. The stressful conditions of manufacturing these drugs can cause protein aggregates to form. These particles are considered undesirable for they can induce an immunogenic response that develops antidrug antibodies, limiting the efficacy of the drugs. Little is known about the exact levels of protein aggregates that cause a heightened immune response. My project involved studying the density of protein aggregates formed by mechanical and thermal stress using particle count, size, and sedimentation data obtained using micro flow imaging measurements. Proteins were stirred, heated, pumped through a syringe, and frozen and thawed to produce aggregates whose characteristics mimic those produced during formulation and delivery of the protein drugs. Beads of controlled shape and known density were first used to determine the accuracy of the measurements. By placing these particles in a narrow tube, they can be magnified and photographed as they fall through fluid using a commercial microscope camera. By analyzing these particles with variable thresholds, a more accurate depiction of size is achieved. Density can then be determined using stokes law by analyzing the tracks of the particles as they fell. The results obtained by this method will be cross checked using Quantitative phase microscopy.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Ebony Cross		**Grant Number**	70NANB16H096
Academic Institution:	Capitol Technology University	**Major:**	Computer Science
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Biosystems and Biomaterials Division, Bioassay Methods Group		
NIST Research Advisor:	Kenneth D. Cole Jamie Almeida		
Title of Talk:	Bioinformatic Analysis for the Standardization of Mouse Cell Line Authentication		

Abstract: Cell line authentication is used extensively in biomedical research and drug development. It is required by FDA for the production of pharmaceutical drugs and is often mandated for publication in journals to ensure the validity of those cell cultures employed. Nevertheless, historically, the frequency of cell line misidentification and cross-contamination has been effectively high. As a result, many of the assumed origins of cell lines used in scientific research and referenced in published papers are inaccurate. The scientific community has confronted the concerns of cell line misidentification and interspecies/intraspecies contamination for human cell lines by creating validated methods to authenticate these cells. While validated procedures to verify human cells lines have been implemented, very few assays exist for nonhuman cell line identification. Consequently, the focus of this research is the design and development of new multiplex polymerase chain reaction (PCR) assays that target specific STR markers found in the mouse genome. This multiplex assay is the first of its kind, providing unique STR profiles for individual mouse samples as a means to authenticate mouse cell lines.

For this project, bioinformatic analysis was conducted on the STR profiles for the individual mouse samples. Data from the Sanger sequenced DNA was then collectively assembled and aligned using the software tool Lasergene SeqMan Pro from the DNASTAR software suite. Lasergene software and electropherograms for the individual samples were used to comparatively analyzed the resulting tetranucleotide sequences of mouse samples. Using Lasergene software, allele mutations, sequence anomalies, and consistency in allele distributions were detected and repeat motifs were determined. Fragment lengths were correlated to actual number of repeats based on the Sanger Sequencing data. These tools are used to characterize and validate the mouse cell line authentication assay. An electronic notebook for completed analysis was created using Microsoft Office suite to create a referential database to be dispersed to the scientific community.

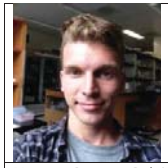
SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Jeremy Filteau		**Grant Number**	70NANB16H162
Academic Institution:	Worcester Polytechnic Institute	**Major:**	Chemical Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Pursuing a career in chemical engineering, hoping to work with pharmaceuticals and drug discovery		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Chemical Sciences Division, Environmental Chemical Sciences Group		
NIST Research Advisor:	Frank Mari		
Title of Talk:	Optimizing preparation methods for venomics analysis of Conus purpurascens		

Abstract:

Marine mollusks of the genus Conus (cone snails) have the ability to synthesize venom to immobilize their prey, which consist of fish, mollusks and worms. Their venom, though tremendously complex, is mainly composed of highly modified peptides – known as conopeptides - that target specific ion channels and cell receptors. These compounds can serve as drug leads for numerous ailments such as neurodegenerative diseases and chronic pain. The analysis of Conus venom is challenging as there is a unique set of conopeptides that can vary greatly between snails of the same species. Sample preparation methods for tandem mass spectrometry introduces further variety in analyzing venom. These protocols, which feature different reagents and techniques, can cause variations in venom data, even if gathered from the same exact snail. It is difficult to identify conopeptide variations in a snail due to crosslinking and modifications. However, the preparation protocol, specifically reduction and alkylation, can be optimized to yield greater coverage of identified conopeptides, improving analysis. Predatory venom was extracted from a *Conus purpurascens* and five reduction and alkylation procedures were tested while the rest of the preparation protocol was kept constant (i.e., sample homogenization and digestion). Methods were evaluated by comparing spectral counts of proteotypic peptides resulting from the digestion via database searching: higher counts indicated more complete reduction and alkylation. The set of reagents and organic solvents that yielded the largest amount of quality matches was deemed the most optimal preparation method for Conus purpurascens analysis. These results will serve as the foundation for future studies optimizing cone snail venom proteomic analysis. A standard preparation protocol will aid in the ability to define the molecular landscape of Conus venom and lead to the discovery of natural product based drugs.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Connor Galvin		**Grant Number**	70NANB16H073
Academic Institution:	Miami Dade College	**Major:**	Biology
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	I plan to finish my undergraduate studies and pursue an advanced degree in hopes of one day conducting research in protein engineering and biocatalysis.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Biomolecular Measurement Division, Macromolecular Structure and Function Group		
NIST Research Advisor:	Travis Gallagher		
Title of Talk:	Exploring a Novel pH-based Strategy for Protein Crystallization		

Abstract:

This project has focused on a major challenge in the field of structural biology -- the low success rate in structure determination due to the difficulty of growing diffraction-quality crystals of a given protein. While most crystals are grown by slowly removing water to induce precipitation, our approach has been to precipitate the protein by gradually shifting the pH to a value where the protein is less soluble. Proteins are polyionic and their solubility is typically a complex multimodal function of pH. The pH can be shifted slowly (over a time course of hours, which is consistent with crystallization) by means of vapor diffusion of acetic acid, which is volatile. Since this method has received little prior attention, we began by measuring the inducible pH shift in a simplified system. We explored the effect as a function of starting and final pH, buffer concentration and concentration of sodium chloride as cosolute. Finally, we applied the method to crystallize the protein lysozyme, by reducing its pH from 5.6 to 4.8 over 6 hours.

SURF Student Colloquium

NIST – Gaithersburg, MD
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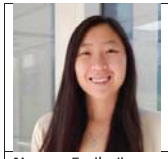
Name: Cristopher Hernandez Macias		**Grant Number**	70NANB16H131
Academic Institution:	Univ MD College Park	**Major:**	Biochemistry
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Planning to pursue either a career in Psychiatry, or a Ph.D. in Neuroscience.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Biomolecular Measurement Division, Bioanalytical Science Group		
NIST Research Advisor:	Lisa Kilpatrick		
Title of Talk:	Observing Trypsin-Catalyzed Transpeptidation Products Using UHPLC-MS.		

Abstract:

Serine proteases, such as trypsin and chymotrypsin, play an important role in the body, in laboratories, and increasingly, in industry. In humans, they are involved in various physiological processes, primarily regulating digestion. In analytical laboratories, they are often used for the characterization of other proteins by mass spectrometry (MS). While in industry, they have been shown to be useful in the manufacturing of new protein products. With novel analytical and bioengineering techniques being used in industry, the need for reliable enzymes will only continue to grow, especially as they begin to be used in the development of biotherapeutics. As such, it is important to continue to expand our understanding of these enzymes, in order to prevent the development of unexpected protein products or unexpected analytical results.

A process that may lead to unexpected protein products during proteolysis is known as transpeptidation, or reverse-proteolysis. This process involves the reversal of catalytic hydrolysis, enabling for new peptides to be synthesized from that enzyme's own hydrolysis products, as well as other peptides present. While this process has been observed *in vitro* since the 1930s, there is much that remains unknown, including its potential impact inside the body, as well as its effects on protein quantification. A major barrier that has prevented further exploration of this topic has been the lack of instrumentation and database search algorithms capable of detecting these transpeptidation products. Throughout the years, researchers have found ways around this and almost always, they have documented this process to occur at higher rates than previously thought.

This project aims to understand transpeptidation through the identification and quantification of trypsin-catalyzed transpeptidation products using UHPLC-MS (Ultra-High-Performance Liquid Chromatography-MS). UHPLC-MS provides both, quantitative and qualitative data with a high degree of resolution and mass accuracy. By limiting the amount of peptides analyzed, transpeptidation products were predicted and closely monitored for various sets of initial conditions; through this, general trends were observed regarding the rate of trypsin-catalyzed transpeptidation. As one of the most commonly used serine proteases, trypsin can reveal much about this general process and the implications it could have inside laboratories and ourselves. Given enough information, transpeptidation could reshape the way we understand proteolysis altogether.



SURF Student Colloquium

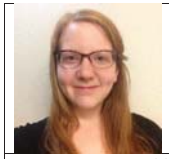
NIST – Gaithersburg, MD
August 2-4, 2016

Name: Emily Jin		**Grant Number**	70NANB16H081
Academic Institution:	Columbia University	**Major:**	Engineering
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	Planning to major in Industrial Engineering/Operations Research and minor in Chemical Engineering		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Biomolecular Measurement Division, Bioanalytical Science Group		
NIST Research Advisor:	Mark Lowenthal Bill Krekelberg		
Title of Talk:	Engineering Biology: Using Bioinformatics to Predict N-Linked Glycosylation Sites in Proteins		

Abstract:

While most people are familiar with the fact that proteins and carbohydrates play an essential role in biology, an understanding of the mechanisms behind the formation of protein-carbohydrate complexes is less widely known. A protein is comprised of a long string of amino acids that partially determines its structure and function. Proteins are often glycosylated – a process in which a carbohydrate binds to a protein. Glycosylation is essential for the folding, function, and stability of the protein. Defects in glycosylation can indicate the presence of many severe diseases, such as cancer. Knowing the location and occupancy rates of specific glycosylation sites can help us diagnose and treat some of these diseases.

In this project, we used bioinformatics to align the amino acid sequences of thousands of proteins to try and predict which potential N-linked glycosylation sites actually become glycosylated based on how well the N-X-S/T/C consensus motif is conserved across species. We theorized that the more highly conserved the consensus motif is at a given site, the more likely that site will become glycosylated. Using Python and its BioPython module, we were able to data mine the UniProt website, a comprehensive database of protein sequences and functional information, for sequences with experimentally proven N-linked glycosylation sites. We then aligned those with the corresponding sequences of other species to perform our statistical analysis. With this data, we can quickly and economically predict the most likely sites of protein glycosylation and apply that knowledge to perform targeted laboratory experiments on select samples.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Emmie Knobloch		**Grant Number**	70NANB16H059
Academic Institution:	Smith College	**Major:**	Biochemistry/Mathematics
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Graduate school, seeking a PhD in chemical and biomolecular engineering or molecular biology		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Biosystems and Biomaterials Division, Biomaterials Cell Group		
NIST Research Advisor:	Diane Bienek		
Title of Talk:	Assessing Standard Assays for Cytotoxicity of Dental Materials		

Abstract:
The cytotoxic effects of all medical devices and materials are a concern, but especially those in dental materials. Fillings and adhesives may remain in the mouth for decades, giving them ample opportunity for any possible cytotoxicity to take effect. Over time, residual uncured resin composite from fillings can leach monomers such as triethylene glycol dimethacrylate (TEGDMA), urethane dimethacrylate (UDMA), and 2-hydroxyethyl methacrylate (HEMA) into the body. Understanding the cytotoxic effects these monomers have on our cells is important for assessing the safety of both novel and existing dental materials.

Current standards for assessing the cytotoxicity of dental materials have been published by several organizations, including the American Dental Association (ADA), the International Organization for Standardization (ISO), and the American Society for Testing Materials (ASTM). These usually involve either placing the solid material or an extract in direct contact with a cell culture or allowing them to diffuse through a filter or layer of agar.

While these standards do provide a reference point for the toxicity of dental materials, they do not accurately represent the environment in which these materials are used. Most suggest the use of animal cell lines, the most common being mouse subcutaneous fibroblasts, and even those that recommend human cell lines generally specify a type of lung cells rather than the gingival cells that materials are most likely to come into contact with. They also expose these cells directly to solid materials that will realistically only ever come in contact with the tooth.

This project aims to provide an alternative to these standards by comparing the response of traditionally tested cell lines like mouse fibroblasts with those of more appropriate human gingival cells. Three cell lines (human gingival keratinocytes, human gingival fibroblasts, and mouse subcutaneous fibroblasts) were exposed to monomers that are known to leach from dental materials (HEMA, TEGDMA, UDMA, and TiO2) in varying concentrations for either 24 or 72 hours. Their cytotoxicity was then measured using metabolic assays and fluorescent live/dead staining. Results indicate that the minimum concentrations at which cytotoxic effects are observed from these monomers are significantly above an amount that could realistically be released, and so are not biologically relevant.

These results will eventually be coupled with the development of a microfluidic device to more accurately simulate gingival tissue and the environment of the oral cavity in which these materials are used, to some degree bridging the gap between traditional in vitro and in vivo testing.

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August 2-4, 2016

Name: Abigail Lee		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland College Park	**Major:**	Chemistry
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Graduate School, University of Maryland, College Park		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Chemical Sciences Division, Organic Chemical Measurement Science Group		
NIST Research Advisor:	Jeanice B. Thomas		
Title of Talk:	Determination of Vitamin C in NIST Food-Matrix Standard Reference Materials		

Abstract:

Well-characterized reference materials and reliable analytical methods are needed in the food testing and nutrition communities to help facilitate compliance with nutritional labeling laws and improve the accuracy of nutrition information that is provided to assist consumers in making sound dietary choices. As a result of the Nutrition Labeling and Education Act (NLEA) of 1990, the National Institute of Standards and Technology (NIST) has developed a series of food-matrix Standard Reference Materials (SRMs) characterized for nutrient concentrations. The NLEA requires food processors to provide specific nutrition information on labels of products distributed in the United States. Information about vitamin C content is required on nutrition labels, thereby making certified reference materials with assigned values for vitamin C useful.

Vitamin C concentrations will be determined in 3 new NIST food-matrix Standard Reference Materials (SRMs) using a liquid chromatographic (LC)-absorbance method developed at NIST. These SRMs include SRM 1869 Infant Formula, SRM 2386 Avocado Powder, and SRM 3233 Breakfast Cereal. The procedure used to extract vitamin C from the different matrices, a description of the LC method employed, and the results from the measurement of vitamin C in each material will be presented.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: Ann Marie Martin		**Grant Number**	70NANB16H058
Academic Institution:	Mount St Mary's University	**Major:**	Chemistry
Academic Standing (Sept. '16):	Graduate Student at American University		
Future Plans (School/Career):	Attend Medical School		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Chemical Sciences Division, Chemical Informatics Research Group		
NIST Research Advisor:	Tom Allison Karl Irikura Peter Linstrom		
Title of Talk:	Optimization of 3D Molecular Structures for the NIST Chemistry WebBook		

Abstract:

The NIST Chemistry WebBook is a widely used resource for scientists, engineers, and students. It is comprised of experimental information such as molecular structure, and spectral data on approximately 140,000 molecules. Our objective this summer is to optimize molecular geometries using Gaussian09, a computational chemistry computer program. Furthermore, we are adding and verifying roughly 20,000 optimized 3D molecules to the WebBook, as well as suggesting changes to the nomenclature and/or 2D structures in the WebBook. The 3D structures are important in areas such as space exploration, experimental simulations as well as drug development.

The 3D structures were optimized using a series of quantum theories ranging from classical mechanics force field approximations to quantum mechanics methods such as Density Functional Theory Method (DFT). First, we utilized the molecular mechanics method (MM2) which gives a cheap approximation of the optimized 3D structure from a 2D drawing. Then, these structures were optimized by the Gaussian program at the semi-empirical PM6 and more accurate B3LYP/6-31g* DFT levels of theory to produce a more accurate result. The B3LYP method is the most accurate method we employ, but also the most time consuming calculation to run and thus is computed last. As the B3LYP method is known to produce reliable molecular geometries, the optimized structures should be in good agreement with the experimental results. After optimization, we verified that the computed 3D structures agreed with the other data in the NIST Chemistry WebBook as well as analyzed the nomenclature, making the appropriate corrections as needed.

Overall, we expect to complete optimization and verification of 20,000 molecules this summer, completing a project to enhance and verify the WebBook that began 5 years ago.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Graham Rich		**Grant Number**	70NANB16H094
Academic Institution:	Virginia Polytechnic Institute and State University	**Major:**	Chemical Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Graduate school		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Chemical Sciences Division, Chemical Informatics Research Group		
NIST Research Advisor:	Nathan Mahynski Vincent Shen		
Title of Talk:	Understanding the impact surface roughness has on gas adsorption		

Abstract: Extensive research has already provided a fundamental understanding of gas adsorption on relatively smooth surfaces, however there is still very little known about how adsorption occurs on rough interfaces. When the adsorbing surface configuration changes, so does the local interaction energy with the gas; this causes the gas particles to adsorb in a non-uniform fashion on the surface. We aimed to study the interaction energy of various different classes of surface features with model gas particles to accurately predict adsorption in porous materials. With the use of several computational models, we have studied the thermodynamic behavior of the adsorption process on different surfaces. We used a python script to simulate a rough surface in order to study the changes in local surface interaction energy as the characteristic geometric features change. To understand how this surface would be different from a smooth interface, we used Monte Carlo (MC) molecular simulations to compute the thermodynamic properties of a model gas in a confined system. Using these programs, we have connected trends in surface geometries to characteristic adsorption behavior. We also studied the density distribution of the confined gas as its pressure varies to investigate the layering effect that occurs at higher pressures inside the pores. We then made comparisons to smooth interfaces. We have now developed a better understanding of the thermodynamics and structure of confined gas particles adsorbed on a rough interface.

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Name: Denis Routkevitch		**Grant Number**	70NANB16H049
Academic Institution:	Johns Hopkins University	**Major:**	Biomedical Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Preparing for MD/PhD to combine research with a career in medicine		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Biosystems and Biomaterials Division, Biomaterials Cell Group		
NIST Research Advisor:	Jeffrey Kim		
Title of Talk:	Analysis of metals in electronic cigarette vapor		

Abstract:
Electronic-cigarettes have been gaining popularity as a supposedly safer alternative to traditional cigarettes. Currently, over 400 companies in the US are selling products with minimal local, state or federal regulations. However, several studies have shown that the e-cigarette vapor contains harmful compounds, including metal nanoparticles that could be released from the heating coil. Additionally, some users have reported sensing a metallic taste from their e-cigarettes after a certain amount of use. Little is known about which metals are present in the vapor, how to quantify those metals, and how they interact with the human body. This study aims to (1) identify metals in the vapor, (2) measure their levels over time and use, and (3) determine the critical point where they may be toxic to humans.

Vapor was produced under published parameters using a standardized e-cigarette testing device filled with e-liquid reference material consisting of propylene glycol, vegetable glycerin, and nicotine with no flavor added. For determination of metal content, the vapor was collected using chilled nitric acid in a gas condenser. A simulated nine days' worth of vapor was collected in each sample for a total of six samples (54 days). The samples were analyzed using inductively coupled plasma optical emission spectrometry (ICP-OES). Silicon, potassium, and magnesium were definitively found in the sample along with trace amounts of copper, calcium, iron, zirconium, and nickel. Many of these have been shown to contribute to upper respiratory irritation. In the near future, this study will quantify the metal content of the samples by comparing their emission peaks with those of standard solutions. Additionally, human oral and lung epithelial cells will be exposed to vapor, collected and analyzed using ICP-OES to determine the cellular uptake rates and pathways of the metals.

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August 2-4, 2016

Name: Angela Rubino		**Grant Number**	70NANB16H061
Academic Institution:	The Citadel	**Major:**	Chemistry and Spanish
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Pursuing a career in environmental science or environmental engineering.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Chemical Sciences Division, Environmental Chemical Sciences Group		
NIST Research Advisor:	Stacy Vander Pol		
Title of Talk:	Exploring Better Methods to Quantify Marine Microplastics for Development of a Standard Reference Material		

Abstract:

While many are aware of the presence of macroplastic pollution and the dangers it poses to the marine environment, microplastic pollution poses a different threat as it is more easily ingested by marine life, and can accumulate toxins. Microplastic contamination may be from released manufactured plastic beads found in stuffed toys and exfoliating soaps, or from macroplastics breaking down into smaller pieces that never fully degrade. An integral part of studying these plastics, is measuring how much microplastic pollution there is in a marine environment, and to do that accurately, a reference material must be developed. To quantify the plastics, they first need to be separated. Currently, separation techniques include density separation with filtration or separating samples using sieves with various mesh sizes then picking out microplastics manually which is tedious, time consuming, and can result in misidentification. We attempted to separate purchased plastics using a density gradient, but due to a narrow density range of all the plastic types, it is impractical to develop a gradient with enough layers to separate them. We also tried separating using a FlowCam based on the size, shape, or color of the plastics; however, there were no definitive differences between each type of plastic. The final separation technique used was gas chromatography mass spectrometry (GC-MS). We were able to find ions unique to plastics of interest and run a selected ion monitoring method against consumer plastics commonly found in a marine environment. The consumer plastics tested, of which the plastic type is known, have been matching our selected ion monitoring method so far. Our current analysis is qualitative; we hope to use this method to quantify a homogenized mixture of plastics as they may be found in a marine environment, and begin development of a Standard Reference Material (SRM) for microplastic quantitation.

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Name: Mariya Shevchuk		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland College Park	**Major:**	Chemical Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Pursuing a career in the biomedical field.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Chemical Sciences Division, Chemical Process and Nuclear Measurements Group		
NIST Research Advisor:	Tom Allison Karl Irikura Peter Linstrom		
Title of Talk:	Optimization of 3-Dimensional Chemical Structures for NIST Chemistry WebBook		

Abstract:

The NIST Chemistry WebBook is a widely used resource for scientists, engineers, and students. It is comprised of experimental information, such as molecular structure and spectral data, on approximately 140,000 molecules. Our objective this summer is to optimize molecular geometries using Gaussian09, a computational chemistry computer program. Furthermore, we are adding and verifying roughly 20,000 optimized 3D molecules to the WebBook, as well as suggesting changes to the nomenclature and/or 2D structures in the WebBook. The 3D structures are important in areas such as space exploration, experimental simulations, and drug development.

The 3D structures were optimized using a series of quantum theories ranging from classical mechanics force field approximations to quantum mechanics methods such as Density Functional Theory Method (DFT). First, we utilized the molecular mechanics method (MM2) which gives a cheap approximation of the optimized 3D structure from a 2D drawing. Then, these structures were optimized by the Gaussian program at the semi-empirical PM6 and more accurate B3LYP/6-31g* DFT levels of theory to produce a more accurate result. The B3LYP method is the most accurate method we employ, but also the most time consuming calculation to run and thus is computed last. As the B3LYP method is known to produce reliable molecular geometries, the optimized structures should be in good agreement with the experimental results. After optimization, we verified that the computed 3D structures agreed with the other data in the NIST Chemistry WebBook as well as analyzed the nomenclature, making the appropriate corrections as needed.

Overall, we expect to complete optimization and verification of 20,000 molecules this summer, completing a project to enhance and verify the WebBook that began 5 years ago.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: Anh Tran		**Grant Number**	70NANB16H159
Academic Institution:	University of Maryland Baltimore County	**Major:**	Biochemistry & Molecular Biology
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Pharmacological Research/Graduate School		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Chemical Sciences Division, Inorganic Measurement Science Group		
NIST Research Advisor:	Lee Yu		
Title of Talk:	How Safe is Our Ginger? A Study of Arsenic Species in Standard Reference Material (SRM 3398) Ginger Rhizome.		

Abstract: Ginger is an indispensable ingredient in cooking and home remedies. With the confluence of popularity of ginger as a dietary supplement and the global sourcing of the commodity, attention is drawn to its safety, and especially to its heavy metal contamination. Arsenic is a toxic and carcinogenic substance that is regularly tested in agricultural products. Arsenic contents in many food and drinks are regulated. However, not all forms of arsenic are toxic. Current regulations focus on the most toxic species of inorganic arsenics: arsenous acid (AsIII) and arsenic acid (AsV). In support of dietary safety measurements of ginger, NIST is developing a standard reference material (SRM) 3398 Ginger Rhizome. However, there is no reported procedure on assessment of toxic arsenic in ginger.

A procedure was developed to reproducibly extract the toxic arsenic species from ginger and then to identify and quantify the arsenic species The extraction procedure was optimized for solvent, temperature, and equilibration time. Arsenic species in the extract were identified based on the retention time of the species, and the quantities were determined by liquid chromatography-inductively coupled plasma mass spectrometry (LC-ICP-MS). Separately, arsenic in the ginger and the ginger extract was determined by ICP-MS for evaluation of extraction efficiency and for validation of the speciation measurement. SRM 3398 was found to contain approximately 50 mg/kg arsenic, of which 4 mg/kg was extracted at room temperature and determined to be inorganic arsenic. Two brands of ginger powder and one fresh ginger from local grocer were found to contain arsenic that were orders of magnitude lower than that in SRM 3398, suggesting that SRM 3398 may not be representative of ginger found in the US market. The amount of extractable arsenic increased exponentially with the temperature, and the implications of this effect will be discussed.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: Aniekanabasi Ufot		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland College Park	**Major:**	Biochemistry/Spanish
Academic Standing (Sept. '16):	University of Maryland graduate		
Future Plans (School/Career):	Pursuing a career in biomedicine		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Chemical Sciences Division, Environmental Chemical Sciences Group		
NIST Research Advisor:	Michael B. Ellisor		
Title of Talk:	Analysis of Trace Elements in Marine Mammal Tissues		

Abstract:

The presence of contaminants in the marine ecosystem is an important concern worldwide. These contaminants negatively impact the health of the marine organisms as well as the health of the local populations that depend on these organisms as a significant source of diet. Exposure to high concentrations of trace elements is a contributing factor to the decline in the population of marine mammals. The Artic marine environment in Alaska is an important geographic location for monitoring as predators such as beluga whales and ringed seals have the potential to accumulate contaminants within their tissues. These predators within the marine food web are good indicator species of the environmental contamination present in the area. The objective of this project is to investigate the concentration of 14 select trace elements (Ag, As, Ca, Cd, Cr, Cu, Fe, Mn, Pb, Rb, Se, Sn, V, and Zn) in liver tissues of ringed seals and beluga whales using inductively coupled plasma mass spectrometry. Tissue samples were obtained from seals and whales ranging from pup to adult in order to analyze any age-related correlations. The results from these analyses will help assess the risk of consuming contaminated food from marine animals as well as contribute to a greater understanding of the impacts of contaminants in the Artic marine ecosystem.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Jessica Young		**Grant Number**	70NANB16H131
Academic Institution:	Univ MD College Park	**Major:** Chemical & Biomolecular Engineering	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Earn a B.S. Degree in Chemical and Biomolecular Engineering		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Biomolecular Measurement Division, Macromolecular Structure and Function Group		
NIST Research Advisor:	Vitalii Silin		
Title of Talk:	Study of Interaction of Peptides with Tethered Bilayer Phospholipid Membranes		

Abstract:
Membrane-lytic peptides exhibit antimicrobial properties and some show selective inhibition of cancerous cells and viruses. These properties of the peptides could prove advantageous in the development of novel antibiotics and chemotherapies. For our study, we chose two peptides: polybia-MP1 (MP1), an antibacterial peptide (found in the venom of the Brazilian wasp) which selectively kills cancer cells over healthy cells, and AH, a synthetic antiviral peptide (derived from the membrane anchor of the hepatitis C virus protein, NS5A) which shows excellent potency to selectively treat flaviviruses, which includes the Zika virus and West Nile virus among others. To understand the mechanisms of action of these peptides, we investigated the interactions of MP1 or AH with model phospholipid membranes of different compositions and degrees of fluidity. MP1 was synthesized, purified using High Performance Liquid Chromatography (HPLC) and analyzed using Mass Spectrometry. As model membranes, we employed tethered bilayer phospholipid membranes (t-BLM) created by rapid solvent exchange. For these studies, we utilized two measurement techniques simultaneously on the same sample substrate: Surface Plasmon Resonance (SPR), an optical technique that measures the amount of peptide and membrane on our sample substrate, and Electrochemical Impedance Spectroscopy (EIS), an electrochemical technique that measures electrical conductance through the membrane and provides information on the presence of defects or pores in our model membrane. We found the combined SPR/EIS technique is an extremely sensitive tool for detecting peptides/membrane interaction. Our data shows that MP1 destroys membranes made from a mixture of (70:30) phosphatidylcholine (PC) and phosphatidylethanolamine (PE) more readily than membranes of (70:30) PC and phosphatidylserine (PS). At high concentrations, MP1 desorbs portions of phospholipids from the membrane. AH, like MP1, caused defects in the membrane, but at a much smaller rate. Unlike MP1, AH did not significantly desorb phospholipids from the membrane at any concentration.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: David Anderegg		**Grant Number**	70NANB16H094
Academic Institution: Virginia Polytech Institute & State University		**Major:** Materials Science and Engineering/Chemistry	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Pursuing a master's degree in Materials Science and Engineering at Virginia Polytechnic Institute and State University		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Chemical Sciences Division, Chemical Informatics Research Group		
NIST Research Advisor:	Daniel Siderius		
Title of Talk:	Developing a System to Encode Multicomponent Adsorption Isotherms for Standard Reference Data Use		

Abstract:

Adsorbent materials have been used for over a century for important applications including gas purification and separation, water purification, and desiccants. In the past two decades, advances in chemistry have led to the development of new adsorbent materials including activated carbons, silicates, and metal organic frameworks. Because of their high surface areas and selectivities, these new materials can be used to develop more efficient and cost-effective methods to remove pollutants from the air, purify solutions, and catalyze reactions. However, due to the extensive number of ways in which they can be modified such as processing temperature, chemical treatment, and composition, they require a substantial amount of research. Currently, there is poor communication between researchers because they lack standardized experimental procedures, material naming conventions, reference adsorption data, and standard formats for data exchange. This has hindered the development of materials capable of solving issues.

A need to improve communication has led NIST to develop a database of Novel and Emerging Adsorbent Materials to aid researchers in accessing and comparing adsorption data. This database is under continuous development and includes only a fraction of the isotherm data that has been published. This summer we helped resolve this issue by digitizing single component isotherms, thereby increasing the reach of the database. Additionally, we expanded the database system to include multicomponent gas adsorption. Multicomponent isotherms are more difficult to digitally encode as the composition of the gas adds constraints that must be recorded to fully describe a multicomponent adsorption experiment. By reviewing several hundred articles on multicomponent adsorption we were able to develop, test, and refine a file format that can robustly and accurately encode this data. This addition is important as it allows for the inclusion of data on selective adsorption of mixtures to represent gases like those found in nature and industry.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: Timothy Barrett		**Grant Number**	70NANB16H
Academic Institution: University of New Hampshire		**Major:** Mechanical Engineer	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Attending graduate school at the University of New Hampshire		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Material Science and Engineering Division, Mechanical Performance Group		
NIST Research Advisor:	Mark Iadicola William Luecke		
Title of Talk:	Uncertainty of the Impulse Excitation Technique		

Abstract:

Accurate measurements of elastic properties in sheet metals allow for a more reliable prediction of the forming of automotive parts. Higher strength materials can reduce vehicle weight and result in better fuel efficiency, but must be properly characterized. For sheet metals, the impulse excitation technique can be implemented to characterize the directional dependence of the elastic properties.

The impulse excitation technique is a non-destructive method that requires only a small amount of material to measure Young's modulus, Shear modulus, and Poisson's ratio. This technique requires meticulous preparation for each specimen and accurate measurement of its mass and physical dimensions. Using a microphone and a resonance frequency analyzer, an impulse is applied to the specimen and its natural frequency is calculated using a Fast Fourier Transform. With these measurements the elastic properties of a material can be determined using vibrating beam or plate theory.

Our goal is to determine if this technique allows for an efficient and accurate measurement of elastic properties compared to complicated static bending and uniaxial testing. Results show that the repeatability depends on key parameters including machining technique, edge condition, supports, and accuracy of micrometer measurements. Limitations and uncertainties of this technique based on geometry and physical measurement capabilities are evaluated allowing for the determination of an optimized geometry for sheet metals. For ease of testing, a 20mm x 50mm x 1mm was selected. Specimens 10mm x 20mm x 1mm can be measured as well, but with a more difficult and time consuming process. After extensive testing a finalized sample preparation and testing technique was selected that can measure Young's modulus repeatedly up to ± 1 GPa and with similar in plane directional dependence seen in static testing.

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Name: Matthew Bleakney		**Grant Number**	70NANB16H159
Academic Institution:	Univeristy of Maryland Baltimore County	**Major:**	Mechanical Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Looking further into graduate school. Possibly following a career dealing with both material science and green energy.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Measurement Science Division, Materials for Energy & Sustainable Development Group		
NIST Research Advisor:	Huong Giang Nguyen		
Title of Talk:	Determining and comparing skeletal density of NIST RM-8852 from different gas measuring techniques/principles		

Abstract:
Gas state molecules play a huge part in today's world, ranging from energy production to greenhouse gas, and when coupled with gas adsorbing materials, we can better manage these resources and mitigate their environmental damages. The ability of a material to adsorb a gas is typically determined from an adsorption isotherm, which is a plot of gas uptake at different gas equilibrium pressures, from which properties, such as surface area, pores size distribution, pore volume, and gas uptake capacity can be derived. While gravimetric and volumetric gas measurement techniques exist, both methods need to account for the sample volume in order to compensate for buoyancy or adjust for dead volume, respectively. The problem lies with the variety of conditions and techniques used to observe the sample volume. Our group aims to investigate the ability of three different gas measurement instruments (helium pycnometer, low pressure volumetric, high pressure volumetric) to measure the sample volumes (and consequently density) of zeolitic Reference Material (RM) 8852, and determine their impact on the resulting gas adsorption isotherms. We will also investigate whether a machine's ability to measure volume will affect the accuracy of other derived data. Currently, we have studied the effects of fill percent and temperature on the helium pycnometer's ability to measure density using Silicon Shot, a non-adsorbing material with a known density. Preliminary results show significant differences in the low pressure volume measurements compared to those from the helium pycnometer, yet this has an insignificant effect on the machine's ability to analyze sample surface area. Our next step is to finish the low pressure experiments and duplicate the low pressure volumetric experiments in the high pressure volumetric system. At high pressure, we expect to see large discrepancies in adsorption isotherms, as errors in volume measurement will be more pronounced.

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Name: Hayley Boigenzahn		**Grant Number**	70NANB16H162
Academic Institution:	Worcester Polytechnic Institute	**Major:**	Chemical Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Graduate school		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Science and Engineering Division, Polymers and Complex Fluids Group		
NIST Research Advisor:	Debra Audus		
Title of Talk:	Using Molecular Dynamics to Investigate the Structure of Polyelectrolyte Micelles		

Abstract:
Under specific conditions, oppositely charged polyelectrolytes in an aqueous enviornment can phase separate into a water-rich phase and a polymer-rich phase through a process known as complex coacervation. If inhomogeneous polymers are used, coacervation can drive self-assembly of complex microstructures. This study primarily concerns diblock copolyelectrolytes, in this case, a neutral polymer covalently bound to a charged polymer. At sufficiently low concentrations, the mixture of oppositely charged diblock copolyelectrolytes forms spherical micelles consisting of a coacervate core with a neutral corona. Since these micelles are responsive to enviornmental factors such as pH and salt concentration, they show potential as drug delivery agents. This study attempts to establish the most favourable aggregation number, or number of polymers in a micelle, for different lengths of neutral and charged blocks through the use of molecular dynamics simulations. A range of systems with different block lengths and aggregation numbers were modelled at infinitely low concentration to establish the existence and stability of a micelle at those conditions. The most favourable micelle size was then determined using free energy estimates via thermodynamic integration. Data from the simulations was also used to explore the radius and concentration of the coacervate core, as well as the diameter of the corona. The core concentration appears to be postively correlated to the length of the charged block but independent of the aggregation number; however, if the charged block is too short the micelle becomes unstable. Such knowledge of these micelle structures helps solidify our understanding of their behavior, which can later be used for research of practical applications. For example, it helps generate better predictions of how the micelles may interact with other molecules, which is important in the case of drug delivery.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: James Boligitz		**Grant Number**	70NANB16H060
Academic Institution:	Temple University	**Major:**	Mechanical Engineering
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Pursuing a career in Mechanical Engineering.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Science and Engineering Division, Thermodynamics & Kinetics Group		
NIST Research Advisor:	Eric Lass		
Title of Talk:	Investigation of phase equilibria in binary Co-W surrounding the μ-phase via mechanical alloying		

Abstract:

Precipitate strengthened Co-based alloys have emerged as a promising material for the next generation of high temperature turbine engine applications. One of the key foundational alloy systems for these alloys is the Co-W binary phase diagram. The goal of this project is to investigate the Co-W phase diagram and, in particular, the compound Co_7W_6, or the μ-phase. To this point, the Co-W phase diagram is well defined in the Co-rich region (less than 20% W by mole fraction), but the area surrounding the μ-phase is still relatively uncertain. Because pure W is the first phase to precipitate from the liquid phase at compositions greater than roughly 35% W, it is difficult to investigate the phase equilibrium below 1650°C. As the alloy is cooled to the temperature range we are interested in (700°C to 1600°C), this nearly pure W remains, and sluggish diffusion does not allow the microstructure to reach equilibrium.

To overcome these issues, mechanical alloying is used to form the Co-W alloy at lower temperatures. Ball milling is used to create an alloy powder with nearly homogenous composition that is cold compacted into a Co-W pellet. The pellet is then annealed at temperatures where the μ-phase forms, in our case 800 °C, 1000 °C, and 1200 °C. The premise is that the homogeneous starting composition combined with the significant plastic deformation energy imparted in the material as a result of ball milling will promote a more rapid approach toward phase equilibrium. Once the pellets are heat treated, the samples are observed using a scanning electron microscope (SEM) with energy dispersive x-ray spectroscopy (EDS) and X-ray diffraction (XRD). These tests are used to investigate the microstructure, phase identification, and phase compositions of each sample.

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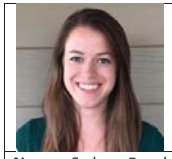
August 2-4, 2016

Name: Preetom Borah		**Grant Number**	70NANB16H055
Academic Institution:	The College of Wooster	**Major:**	Chemistry/Music
Academic Standing (Sept. '16):	Recent graduate of The College of Wooster		
Future Plans (School/Career):	To gain work experience in a government or industry lab before attending graduate school		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Measurement Science Division, Microscopy & Microanalysis Research Group		
NIST Research Advisor:	Thomas Forbes Edward Sisco		
Title of Talk:	Optimization of thermal desorption direct analysis in real time mass spectrometry (TD-DART-MS) for the detection of illicit narcotics		

Abstract:

The detection of contraband materials such as narcotics and explosives is of continued importance in forensics, safety and security. Laboratory methods used for detection include ion mobility spectrometry (IMS), surface-enhanced Raman scattering (SERS), and ambient ionization mass spectrometry (MS) among others. Here, one such ambient ionization method, Direct Analysis in Real Time (DART), was coupled with thermal desorption (TD) in a confined geometry for the detection of contraband materials. This coupling provides a high sensitivity and selectivity technique for the rapid analysis of swipe samples, a common sampling method in forensic and security arenas, relevant to the border patrol, law enforcement, and prisons. Initial studies investigated two main parameters of the TD-DART-MS system, specifically desorption temperature and the gas/analyte transport flow rate (the rate at which desorbed material was pulled through the confined geometry toward the mass analyzer). Illicit narcotics, including, methamphetamine, heroin, THC, MDMA, cocaine, and MDPV were pipetted onto DSA detection traps (PTFE-coated fiberglass weave) and directly analyzed for parametric studies. Optimal desorption temperatures and transport flow rates were identified for each narcotic as well as the overall range of compounds. The optimized system was then used to investigate the MS response of analyte distributions using precise inkjet printing deposition. Specifically, the signal of THC was measured as a function of array size, representing the differences analyte particle size and surface coverage play for equivalent total mass – increasing array size represented increased number of smaller particles across a larger area. These studies demonstrated an increase in both overall signal intensity and rate of desorption as the array size was increased. Demonstrating the utility of this sensitive and selective technique, the results provided intricate details of the desorption process and a look into the importance analyte distribution and particle size (not simply overall mass) play in overall sensitivity and quantification of compounds.



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NIST – Gaithersburg, MD
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Name: Sydney Brooks		**Grant Number**	70NANB16H158
Academic Institution:	West Virginia University	**Major:**	Chemistry and Forensic Science
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Planning on attending graduate school for forensic chemistry		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Measurement Science Division, Security Technologies Group		
NIST Research Advisor:	Amanda Forster		
Title of Talk:	Fiber Trace Evidence: Quantification of Sample Bleaching During UV-vis Microspectrophotometry		

Abstract:

Textiles are mass-produced around the world and used in many different ways. Consequently, textile fibers are one of the most common types of trace evidence recovered from crime scenes. Identifying and matching a fiber to a known source is a difficult task, and the final conclusion is often accompanied by a significant degree of uncertainty. Fiber examiners often have limited resources and heavy caseloads, further complicating the investigative process. The National Institute of Standards and Technology has taken on multiple projects pertaining to the examination of fibers with the goal of simplifying and standardizing forensic fiber examination. This particular project focuses on one of the most common methods for analyzing fiber color, measuring the absorption of electromagnetic radiation in the ultraviolet-visible light (UV-vis) region using a microspectrophotometer (MSP). However, due to the fact that the instrument utilizes UV light, extended exposure while the fiber in under the microscope can lead to bleaching of the sample. The bleached color then affects the data and can prevent the examiner from being able to make a definitive match between unknown and known fibers. The goal of this research is to quantify the bleaching over time in order to provide guidelines for interpreting data when extended time under the MSP cannot be avoided.

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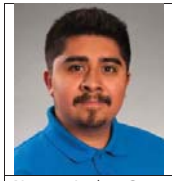
NIST – Gaithersburg, MD
August 2-4, 2016

Name: John Collini		**Grant Number**	70NANB16H091
Academic Institution:	Rochester Institute of Technology	**Major:**	Physics/Math
Academic Standing (Sept. '16):	Graduate Student: University of Maryland, College Park		
Future Plans (School/Career):	Pursuing a career in condensed matter physics/engineering in either government or industry.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Measurement Science Division, Nanomechanical Properties Group		
NIST Research Advisor:	Brian Bush Richard Gates		
Title of Talk:	Nanomechanical time-dependent properties of PEG Hydrogels		

Abstract:

Hydrogels have become attractive materials for use in biomedical and biomechanical fields for their ability to function like natural tissues and act as biological scaffolding. Their biocompabiable nature and material characteristics make them ideal candidates for use in tissue engineering and drug delivery methods. To better understand their mechanical properties for use in these applications, time-depedent nanomechanical load testing experiments are performed on poly(ethylene glycole) (PEG) hydrogels of varying PEG weight concentation *via* a Au colloidal atomic force microscope (AFM) probes. During experimentation, the gels are indented to a maximum load ranging from 5 nN to 20 nN and then subjected to a displacement-controlled hold period for 30 seconds. The load-relaxation response during the hold period is captured and modeled to extract time-dependent visco- and poroelastic mechanical properties. The knowledge gained here will assist future researchers in measuring nanomechanical properties of their hydrogels, as well as, provide the specifications needed for future biomedical engineered devices.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Andres Correa Hernandez		**Grant Number**	70NANB16H045
Academic Institution: Boise State University		**Major:** Materials Science & Engineering	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Obtain a Ph.D. in Materials Science & Engineering		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Measurement Science Division, Materials Structure & Data Group		
NIST Research Advisor:	Eric Cockayne		
Title of Talk:	Density Functional Theory Studies of Nanoporous Materials		

Abstract:

Carbon capture and sequestration (CCS) technologies aim to reduce the ever-increasing carbon emissions entering the atmosphere from coal-burning power plants. The advances that have been made in the field of nanoporous solids make these types of materials excellent candidates for innovative solid-CCS technologies which can, in principle, sequester carbon with less energy compared to currently implemented liquid-CCS technologies. Metal-organic frameworks (MOFs) consist of metal ions bridged by organic linkers, held together by a coordinated covalent network, forming finely tuned nanopore arrays. The flexibility and control of the MOF pores give unique adsorption and desorption affinity towards selected gases. It is the fine control of the nanoporous materials which also gives rise to many possible MOF structures and configurations.

Two MOFs of interest, Ni(1,2-bis(4-pyridyl)ethylene)[$Ni(CN)_4$] and Cu-1,3,5-benzenetricarboxylate, or $Ni_2(CN)_4$-bpene and Cu-BTC respectively, were investigated through density functional theory (DFT) calculations using the Vienna ab-initio simulation package (VASP). Scripts were devised to generate multiple configurations for the $Ni_2(CN)_4$-bpene structure with different orientations of the bpene molecules, as well as for positioning of CO_2 molecules in the Cu-BTC pores. The DFT calculations used to solve the electronic structure for these configurations ran in parallel on a computer cluster. The van der Waals' interactions in $Ni_2(CN)_4$-bpene play an important role in determining the structure. A candidate structure is found for the as-yet unknown structure of empty $Ni_2(CN)_4$-bpene. In Cu-BTC, the rigidity of the Cu-BTC pores makes structural relaxation studies simpler. Hence, analyzing the interactions of CO_2 guest molecules with the pores becomes readily accessible through a DFT approach.

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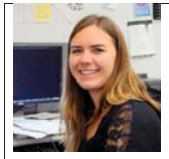
August 2-4, 2016

Name: Anushka Dasgupta		**Grant Number**	70NANB16H054
Academic Institution: Princeton University		**Major:** Chemical & Biological Engineering	
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	Graduate school		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Science and Engineering Division, Mechanical Performance Group		
NIST Research Advisor:	Jonathan Guyer Yannick Congo Daniel Wheeler		
Title of Talk:	Evaluating the Accuracy of Phase Field Codes Using Community-Developed Standard Benchmark Problems		

Abstract:

The phase field method (PFM) is used to model phase transitions at the mesoscale. It is widely used and developed in the materials science community to characterize the dynamics of processes such as grain coarsening and solidification. The PFM has been implemented in numerous ways - in fact, there are dozens of codes available for solving PFM with a variety of capabilities and limitations. Recently, the PFM community reached agreement and published an initial set of benchmark problems to compare phase field codes so practitioners can make sensible choices when selecting codes.

In this work, two of the benchmark problems are implemented (spinodal decomposition and Otswald ripening) in two well established phase field codes -- FiPy and MMSP -- and then compared with the results from a third phase field code -- MOOSE. The work establishes metrics and a workflow for comparing the codes on each of the benchmark problems. The workflow for each comparison is annotated in a Jupyter Notebook for inclusion in the CHiMaD phase field website to encourage other PFM practitioners to evaluate and include further PFM codes on the website. The work mainly addresses the accuracy of the implementations, not the computational efficiency of each code. In particular, the free energy evolution is compared for each benchmark problem at different grid sizes to determine an order of accuracy. Further work by another SURF student uses the generated notebooks to capture metadata, including the computational efficiency, from each simulation.



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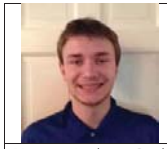
NIST – Gaithersburg, MD
August 2-4, 2016

Name: Aline Elquist		**Grant Number**	70NANB16H045
Academic Institution: Boise State University		**Major:** Materials Science & Engineering/ Physics	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Science and Engineering Division, Mechanical Performance Group		
NIST Research Advisor:	Jonathan Guyer		
Title of Talk:	New Models for Electrochemical Systems		

Abstract:

One of the biggest challenges associated with renewable resources is energy storage and transfer. Developing devices to solve these problems, such as batteries and fuel cells, require improved models of electrochemical systems. Predicting the charge at the interface is necessary for accurate modeling of electrochemical reactions, and design of improved catalysts. The complex interplay between the ion, dielectric, and electrode make accurate models of the change in charge with voltage, or differential capacitance, difficult to produce. Attempting to create a more comprehensive picture, we used two different modeling techniques to simulate measurements of differential capacitance. Our first approach combines density functional theory with a continuum solvation model. Density functional theory uses the electronic structure to calculate the free energy at the ground state of the system. Our second model uses a phase field technique to capture the charge separation at equilibrium at the electrochemical interface. Phase field is derived from continuum thermodynamics and measures the microstructural evolution at the mesoscale. The two models use different approaches to simulate the same measurements. We calculate surface charge and differential capacitance as functions of potential from both models, and compare the results to each other, as well as those found in experiment.



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NIST – Gaithersburg, MD
August 2-4, 2016

Name: Andrew Gayle		**Grant Number**	70NANB16H046
Academic Institution: Duke University		**Major:** Mechanical Engineering and Materials Science	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Graduate school – unknown location; followed by work in a research lab		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Measurement Science Division,		
NIST Research Advisor:	Robert Cook Chris Michaels Brian Bush		
Title of Talk:	Nano-Scale Strain Mapping in Three Dimensions		

Abstract:

Strain (or stress) engineering is used in many advanced devices to optimize properties. Examples include strain engineering channels with enhanced conductivity in microelectronics as well as strain engineered membranes with enhanced stiffness in microelectromechanical systems (MEMS). To achieve such properties, nano-scale strain mapping is required to optimize strain magnitude and location. This project uses nanoindentation flaws as test vehicles for developing strain measurements and mapping methods in three dimensions, expanding on prior NIST strain mapping achievements in two dimensions. Commercial nanoindenters are used to create flaws in samples, in this case single crystal silicon with different crystallographic orientations [(100), (110), and (111)]. Single crystal silicon is a predominant material in MEMS and microelectronic devices. Atomic force microscopes (AFMs) are used to accurately measure the resulting surface profiles with high confidence. In order to generate strain maps, NIST custom Raman and electron microscopes are used to perform Raman Piezospectroscopy and Electron Backscatter Diffraction (EBSD), respectively. By integrating these two techniques with surface profiles, one can validate the resulting strain maps.

Thus far, each of these measurements and techniques have been performed on several single crystal silicon (100) samples. Initially some problems persisted with indenter tips, indenter head alignment, and cleanliness of the samples. These have each been resolved to a satisfactory degree. In terms of analysis, strain maps generated from EBSD and Raman Piezospectroscopy appear accurate and promising. Correlating these strain maps with surface profiles obtained using an AFM will soon follow. In the future, measurements will be taken for the (110) and (111) samples.

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NIST – Gaithersburg, MD
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Name: James Gayvert		**Grant Number**	70NANB16H074
Academic Institution:	Le Moyne College	**Major:**	Chemistry and Computer Science
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Intends to pursue an advanced degree in the field of chemistry.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Science and Engineering Division, Polymers & Complex Fluids Group		
NIST Research Advisor:	Alexandros Chremos Jack Douglas		
Title of Talk:	Molecular Dynamics Study of the Conformational Properties of Polymers in an Explicit Solvent and the Identification of the θ-Temperature		

Abstract:

Numerous biological processes that are critical for life involve polymers in aqueous solutions, and it is important to understand the changes in polymer shape that take place due to variation of thermodynamic conditions and applied perturbations such as flow. Many polymer models are developed with an implicit solvent, rendering these models less useful for the study of such off-equilibrium phenomena. Inspired by the nature of these biological processes, we use a coarse-grained bead-spring model with an explicit solvent to identify the θ-temperature of polymers of different molecular architectures at equilibrium, with the intention of later using this model to simulate the behavior of polymer solutions in off-equilibrium conditions more akin to those we see in nature. The conformational properties of a polymer chain in solution depend on the quality of the solvent, which varies with temperature and chemistry. In a good solvent, the effective interactions between the polymer segments are repulsive, causing the chain to swell in order to maximize polymer-fluid interactions. On the other hand, in a poor solvent the effective interactions between segments are attractive, causing the chain to collapse. At the θ-temperature, the attractive and repulsive interactions between polymer segments cancel each other out, resulting in the polymer conformation having dimensions that of a random walk. The θ-temperature is of particular interest to scientists, because these conditions mark the boundary between polymers exhibiting a tendency to remain in solution versus exhibiting a tendency to precipitate. In this molecular dynamics study, linear chains, rings, and branched polymers of varying molecular masses and chemistries are modeled with a bead-spring model in an explicit solvent. The generated trajectories are investigated with the ZENO numerical path integration package to obtain the conformational properties of these polymers such as the radius of gyration, hydrodynamic radius and diffusion.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Lorelis González López		**Grant Number**	70NANB16H161
Academic Institution:	University Of Puerto Rico - Mayagüez	**Major:**	Chemical Engineering
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	My plan is to attend graduate school to continue my education in the Material Science and Engineering field.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Science and Engineering Division, Functional Polymers Group		
NIST Research Advisor:	Christopher Liman		
Title of Talk:	Using capillary force lithography to make oriented polymer nanogratings		

Abstract:

Polymer nanostructures with molecular orientation have a wide range of applications, including in organic electronics and in next generation lithography techniques. In order to take full advantage of these materials, their morphologies and molecular orientations must be precisely analyzed and understood. To achieve this, nanopatterned polymer gratings were fabricated with the goal of achieving more consistent and homogeneous morphology and strong molecular orientation. Composite polydimethylsiloxane (PDMS) stamps were first prepared following a previously established procedure. The stamps consisted of a thin hard-PDMS layer, supported by a thick slab of soft-PDMS. The fabrication procedure was optimized by varying certain parameters, such as the solvent used and the spin coating conditions (solution volume and rotation speed). Nanopatterned polymer gratings with biaxial anisotropy were then made using these PDMS stamps. The pattern was transferred from the stamp to the sample by solution capillary force lithography. To obtain a homogeneous pattern transfer, various conditions of the procedure were varied. These included the amount of polymer solution used and the direction in which the stamp was placed above it. Atomic force microscopy was used to verify the morphology of both the PDMS stamps, and the nanopatterned polymer gratings. The molecular orientation of the polymer nanogratings was studied using spectroscopic ellipsometry, and polarized ultraviolet–visible spectroscopy.

SURF Student Colloquium

NIST – Gaithersburg, MD
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Name: Sarah Hood		**Grant Number**	70NANB16H136
Academic Institution:	Hood College	**Major:**	Mathematics
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	I plan to pursue a master's degree in a Mathematics field.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Science and Engineering Division, Thermodynamics & Kinetics Group		
NIST Research Advisor:	Benjamin Burton Carelyn Campbell Yannick P. Congo		
Title of Talk:	Domain Structures and Dynamics of Polar Ordering in $Pb(Sc_{\frac{1}{2}}Nb_{\frac{1}{2}})O_3$ with Pb-O Divacancies		

Abstract:

Ferroelectrics are materials that exhibit spontaneous electric polarization, which can be reversed by the application of an external electric field. Chemical disorder and/or short-range order in relaxor ferroelectrics creates a low-temperature polar microstructure that is characterized by nano-scale polar domains, and exhibits no macroscopic polarization. Relaxor ferroelectrics have incredible dielectric and electromechanical properties that make them attractive for real life applications such as ultrasonics, energy harvesting, signal processing devices, transducers and actuators. The goal of this research is to simulate, characterize, and understand relaxor domain structures and their dynamics; most importantly including the glassy freezing of domains at low temperatures. In conclusion, the results found are shown in simulation movies that were made at various temperatures, and they show that polar ordering is strongly correlated with chemical order, even at high temperatures. More results were found in graphs of the average temporal correlation functions which shows the glassy regions are present around the 200K temperatures identified by unsmooth plot points.

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Name: Heetae Jeon		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland College Park	**Major:**	Chemical & Biomolecular Engineering
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Plan to pursue career in polymer science		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Biosystems and Biomaterials Division, Biomaterials Cell Group		
NIST Research Advisor:	Jirun Sun		
Title of Talk:	The Unique Functions of Urethane dimethacrylate in Photo-copolymerization with an Ether-based Divinylbenzyl Monomer		

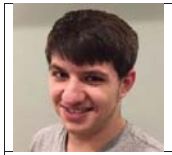
Abstract:

Objective: Ester-based dental resin composites are the dominant restorative materials in treating dental caries, but their average service life is only 7 years due to ester decomposition and secondary caries. Ether-based monomers were invented to replace the dimethacrylate resins because they are hydrolytically and enzymatically stable. However, the polymerization of vinylbenzyl groups was slow to be used in dental clinic. The objective of this research is to enhance the polymerization rate of triethylene glycol divinylbenzyl ether (TEG-DVBE) and understand the kinetics and mechanism of the polymerization process.

Materials and Methods: Real time Fourier transform infrared spectroscopy (FTIR) equipped with Attenuated Total Reflectance (ATR) was used to evaluate the kinetics of polymerization. Urethane dimethacrylate (UDMA), ethoxylated-bisphenol-A-dimethacrylate (EDMA), bisphenol A-glycerolate dimethacrylate (Bis-GMA), and TEG-DVBE were homo-polymerized with either camphorquinone (CQ)/ethyl 4-dimethylaminobenzoate (4E) in 0.2 wt% to 0.8 wt% or Irgacure 819 (I819) in 0.5 mol% as photoinitiators. All the samples were cured for 20 seconds with blue light at 400 mW/cm^2. Each dimethacrylate was also copolymerized with TEG-DVBE in equimolar ratio. After processing the FTIR spectra with Fityk, the degree of vinyl conversion (DC) was determined by monitoring the reduction of -C=C- stretching peak heights using -N-H- (Amide II) as an internal standard. The composition of the copolymer was determined based on the ratio of the remaining monomers.

Results: The polymerization rate of TEG-DVBE was significantly improved by copolymerizing with dimethacrylate monomers. After copolymerization with UDMA for five minutes, the DC was approximately 57 % (±3 %) with CQ/4E and 61 % (±0.5%) with I819 as initiators, respectively. After an hour, both system achieved about 70 % DC. TEG-DVBE polymerized faster with UDMA than it did with EDMA or BisGMA when CQ/4E was used. In addition, the composition of the UDMA/TEG-DVBE remained constant during the polymerization process, while composition shift was observed when TEG-DVBE was copolymerized with EDMA or BisGMA. The functions of UDMA as coinitiators were furthered confirmed by homo-polymerizing UDMA without the presence of 4E. The DC of UDMA reached the same level with and without 4E by varying the amount of CQ, while other dimethacrylate monomers did not cure without 4E.

Conclusion: The copolymerization results suggest that UDMA may serve as a co-initiator with CQ, while other dimethacrylates do not. The unique function of UDMA during copolymerization includes increasing the polymerization rate and controlling the composition of the copolymer. UDMA and TEG-DVBE copolymer system could serve as a longer-lasting dental resin.



SURF Student Colloquium

NIST – Gaithersburg, MD
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Name: Joseph Lagnese		**Grant Number**	70NANB16H159
Academic Institution:	University of Maryland Baltimore County	**Major:**	Computer Science / Mathematics
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	I plan to obtain a Master's Degree in Computer Science from UMBC, and am strongly considering pursuing a PhD. I will likely specialize in cybersecurity and/or software design.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Measurement Science Division, Materials for Energy & Sustainable Development Group		
NIST Research Advisor:	Marcus Mendenhall		
Title of Talk:	Analyzing the Analyzer: A Monte Carlo Investigation of X-Ray Diffraction Fits Generated by TOPAS5		

Abstract:
In order to analyze the atomic structure of crystals, a technique known as X-ray diffraction is often used. With this method, a crystal is aligned with a given X-ray source and illuminated with X-rays. These X-rays diffract off the crystal, producing a unique pattern of reflections which can be cross-referenced with known patterns to determine the structure of the crystal. For our project, we analyze the reflections using a "fundamental parameters" approach where we attempt to fit the pattern using a function which has many parameters which are physically grounded to the crystal and instrument. To generate this fit, we use a highly popular piece of software known as TOPAS5 which uses a very finely-tuned least-squares fitter. It is a common challenge in non-linear least-squares regression to find the true global minimum for χ^2—programs often get caught in local minima and are unable to "find a way out." This means that TOPAS runs the risk of not generating the best possible fit for the data. For this project, we examined whether or not TOPAS always reaches the best possible model depending on its initial parameters, or if the program even generates the best possible fit at all. To this end, we performed a Monte Carlo analysis of TOPAS by providing it with thousands of randomized initial fit conditions for each data file to determine whether it eventually reached the same fit regardless of its initial parameters. Through our research, we found that multiple parameters which were being represented as having approximately normal distributions had distinctly non-Gaussian (non-normal) distributions. We also found some parameters which were bimodal, and found unexpected correlations between some of the variables we examined. Our findings suggest that the goodness-of-fit which TOPAS reaches, while optimistic, can still vary to a fair degree depending on its initial fit.

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August 2-4, 2016

Name: Erica Lee		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland College Park	**Major:**	Materials Science & Engineering
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Measurement Science Division, Security Technologies Group		
NIST Research Advisor:	Aaron Forster		
Title of Talk:	Durability of Carbon Nanotube Reinforced Alumina Fiber - Epoxy Composites		

Abstract:
Fiber reinforced composites are often used as structural elements in aerospace, transportation, and energy applications due to their high strength to weight ratio. Unfortunately, traditional fiber reinforced plastic composites are prone to failure due to out-of-plane loading via delamination and matrix cracking. Multiwalled carbon nanotubes (CNTs), attached directly to the reinforcing fibers, have been shown to significantly improve out of plane fracture toughness and interlaminar shear strength. These improvements have been attributed to the nanotubes' ability to increase the energy required for crack propagation through the epoxy matrix. However, there are few studies on the durability of these CNT modified fiber composites.

A durability study was performed by immersing CNT and non-CNT reinforced alumina fiber-epoxy composites in water at 25 C and 60 C up to 90 days. Mechanical and chemical changes in the composites were characterized through a 3 point bend test combined with acoustic emission and electrical resistance monitoring, water uptake measurements, X-Ray diffraction, and SEM imaging.

We found that there was no change in strength at ambient conditions. On the other hand, the alumina composites exhibited a loss in flexure strength and absorbed more water than the CNT composites at the elevated temperature. FTIR and X-ray diffraction confirmed the presence of $Al(OH)_3$ peaks on the outer alumina fiber surfaces. Dry alumina fibers absorb water, causing the formation of oxide hydroxides. These oxides weaken the bonding between the fiber and polymer, thereby reducing the composite's mechanical strength. While the nanotubes did not prevent alumina hydration, CNT reinforcement prevented strength reductions as the composite degraded. The impacts of this research on applications of CNT reinforced fiber composites will be further discussed.

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Name: Michael Locke		**Grant Number**	70NANB16H051
Academic Institution:	University of New Hampshire	**Major:**	Mechanical Engineering
Academic Standing Sept. '16):	Junior		
Future Plans (School/Career):	I plan to attend graduate school to further my studies in the field of Mechanical Engineering		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Science and Engineering Division, Mechanical Performance Group		
NIST Research Advisor:	Steven Mates		
Title of Talk:	Characterizing Material Behavior Via High-Rate Mechanical Testing Using a Split Hopkinson Pressure (Kolsky) Bar and Pulse Heating System		

Abstract:

To accurately simulate rapid deformation processes such as forming, impact welding, and subtractive manufacturing, we need to understand how materials behave at high strain rates and, usually, elevated temperatures. Efforts during this fellowship included the characterization of 1018 steel, 6061 Aluminum, and 1100 Aluminum, which are currently being examined as part of rapid deformation research at the University of New Hampshire. The typical method used to measure high strain rate mechanical properties is a Split Hopkinson Pressure (Kolsky) Bar. In this work, I use a specialized Kolsky bar method that is outfitted with a pulse heating system to perform tests over a range of temperatures. This form of material testing provides measurements of stress, strain, strain rate, and temperature. These measurements are then used to calibrate the Johnson-Cook flow stress model, which is a popular and simple empirical model of material strength at high strain rates and temperatures that can be used to simulate rapid deformation processes being examined at the University of New Hampshire.

Mechanical measurements were performed on these materials at strain rates between 2000 s^{-1} and 4000 s^{-1}, and temperatures from 23°C up to about 100°C below the melting point. Johnson-Cook model coefficients were obtained by finding the lowest deviation between the model data and experimental data using a customized MATLAB script that I developed. The results of the fitting showed good agreement with the data for 6061 Al and for steel up to about 400°C. However, the Johnson Cook model was unable to capture the steel behavior above this temperature due to dynamic strain aging and phase transformation phenomena in this material, revealing the fact that this simple model cannot capture many real material effects.

"The Future Belongs to Those Who Believe in the Beauty of Their Dreams"

- Eleanor Roosevelt

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August 2-4, 2016

Name: Norman Luu		**Grant Number**	70NANB16H160
Academic Institution:	Northwestern University	**Major:**	Materials Science and Engineering
Academic Standing (Sept. '16):	5th year in a BS/MS program in Materials Science		
Future Plans (School/Career):	Ph.D. in Materials Science and Engineering		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Science and Engineering Division, Thermodynamics & Kinetics Group		
NIST Research Advisor:	Lucas Hale Zachary Trautt		
Title of Talk:	Property Calculations Within the Interatomic Potentials Repository Framework		

Abstract:
Molecular dynamics (MD) is a quick and inexpensive computational method that can describe both the kinetic evolution of an atomistic system and its thermodynamically favorable states. However, MD results depend largely on the interatomic potentials used to define the energy landscape of the system. With this in mind, NIST actively maintains the Interatomic Potentials Repository (IPR), which hosts dozens of potentials for various elements and elemental compounds. That said, it is often difficult for researchers to determine which potential is most appropriate to use. A solution is to use standardized Python scripts that can aid high-throughput screening of potentials while also allowing users to vary values for different computational parameters. Versions of these scripts have already been developed to model point defects and dislocations in crystals, and in support of this ongoing project, we have developed modular scripts to calculate surface energy, generalized planar fault energy, and Bain transformation energy landscapes. We will demonstrate the use of the Python notebooks, discuss the calculations as implemented, and discuss plans to integrate them into the IPR framework.

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Name: Gordon McCann		**Grant Number**	70NANB16H042
Academic Institution: Gettysburg College		**Major:** Physics	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Attend graduate school		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Chemical Sciences Division, Chemical Informatics Research Group		
NIST Research Advisor:	Harold Hatch Nathan Mahynski		
Title of Talk:	Simulation of Superquadric and Supertoroid Particles to Examine the Effects of Particle Shape upon Self-Assembly Behavior		

Abstract:

This talk discusses the development of a Monte Carlo simulation of three dimensional particles, which are defined superquadrics and supertoroids, to examine self-assembly and particle packing behaviors of real world particles with a wide variety of shapes, such as red blood cells or proteins. A superquadric is an object defined by a set of parametric equations which can represent shapes such as cubes, cylinders, or spheres. A supertoroid is similar to a superquadric, but has a hole in the middle. This work focuses on the extension of existing particle interaction simulation of identical superquadrics to include supertoroid particles and non-identical particles. This could lead to an increased understanding of binding sites for proteins, phase transitions, or development of new materials from self-assembly behavior.

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Name: Andrey Moskalenko		**Grant Number**	70NANB16H101
Academic Institution: Purdue University		**Major:** Physics/Environmental and Ecological Engineering	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Attend grad school for either Mechanical or Environmental Engineering, pursuing research related to renewable energy.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Science and Engineering Division, Thermodynamics & Kinetics Group		
NIST Research Advisor:	F. Yannick Congo Carelyn Campbell Daniel Wheeler		
Title of Talk:	Developing the Cloud of Reproducible Records (CoRR) and evaluating its performance compared to existing tools.		

Abstract:

Due to the irreproducibility of computational research, there has been a recent push for a reliable, automated, and effective method of capturing simulations. Thus, the scientific community has seen the appearance of tools such as mercurial and Git for source code version control; Sumatra for execution control; virtual machines, docker and ReproZip for environment control; tavern and galaxy for workflow control. Each of these tools is appropriate for very different needs, however they are not integrated with each other or other systems. We are working to develop a tool called the Cloud of Reproducible Records (CoRR). The goal is to integrate various systems such as version control, environment control and possibly workflow control with a new system of tracking simulation execution, and uploading reproducible records to the cloud platform counterpart of the project. This way a scientist has the ability to collaborate by downloading a record, then rerun it to get the same results or modify it to extend their own research.

We were able to make progress by developing simple phase-field benchmark problems which simulate the phase transitions between materials. These benchmark problems would serve as a way to determine how the previously mentioned systems of execution control perform. Then we replicate the effective features, and incorporate new features such as cloud storage and more intensive metadata tracking. Once CoRR is complete, it will enable users to easily identify causes of failures, crashes and result variations. Users could also perform extensive parameter studies all while CoRR autonomously ensures that the research is reproducible and easily sharable with others.

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NIST – Gaithersburg, MD
August 2-4, 2016

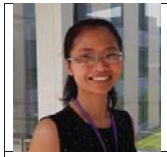
Name: Kathleen Mullin		**Grant Number**	70NANB16H044
Academic Institution:	Illinois Institute of Technology	**Major:**	Materials Science and Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	After finishing my undergraduate degree, I plan to go to graduate school.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Office of Data and Informatics,		
NIST Research Advisor:	Kimberly Tryka Chandler A. Becker		
Title of Talk:	Enabling Discovery of Materials Science Resources Through Robust Metadata Records		

Abstract:
"What materials data is available for my project, and how do I find it?" With the increasingly large amount of materials science data being produced, that question is being asked by researchers every day. Because more and more data is being generated, researchers still have difficulty locating and obtaining the data they need.

To address this problem, NIST began work on a registry system that will enable a worldwide network of materials-related data resources to be cataloged and made more discoverable, accessible, and searchable. This registry system, the NIST Materials Resource Registry (NMRR), is organized into categories, such as data collections, data sets, organizations, informational pages, services, and software. All of the resources have shared metadata (information about the data) that is the same regardless of type (e.g., identity and publication information), and some types of resources have additional fields that are specific to that resource.

My project focused on developing materials-related content for the registry and providing user feedback from a materials scientist in order to make improvements in functionality and the interface. To gain familiarity with the system, I began by examining the resources that were already in the registry and then revised and expanded many of the existing records. I subsequently gathered metadata to create new registry records.

Once I was familiar with the system, I worked on migrating resources from the existing MGI Code Catalog to an instance of the materials resource registry as a way to increase the accessibility of those records. However, the existing NMRR and Code Catalog schemas (resource descriptions) were not the same. To help merge the two different descriptive structures, a careful comparison between the two was completed, noting the similarities and differences. Once this comparison was done, a merged specification that retained the information from both systems was created. This migration will significantly enhance the value of both the MGI Code Catalog and the NMRR.



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NIST – Gaithersburg, MD
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Name: Ai Nguyen		**Grant Number**	70NANB16H
Academic Institution:	Montgomery College	**Major:**	Biochemistry
Academic Standing (Sept. '16):	University of Maryland, College Park, sophomore		
Future Plans (School/Career):	I plan to pursue a career in toxicology or organic synthesis		
NIST Laboratory, Division, and Group:	Material Measurement laboratory, Materials Science and Engineering division, Functional Polymers group		
NIST Research Advisor:	Christopher Stafford, Bradley R. Frieberg		
Title of Talk:	A performance of water and light: Characterizing water purification membranes using ellipsometry		

Abstract:

Polymer has become an essential material in everyday use, especially in the water purification industry. A thin polymer layer (≈100 nm) acts as a permselective membrane that separates salt ions from water. The conventional method in fabricating this active layer is interfacial polymerization due to its scalability and simplicity. However, the chaotic polymerization process prohibits a detailed understanding the membrane's structure and transport. Solution-based molecular-layer-by-layer (mLbL) film growth overcomes this problem by enabling nanoscale control of the selective layer thickness and roughness, but slow film formation and the use of volatile solvents make it undesirable in manufacturing. As a result, NIST researchers are working with the University of Colorado on a vapor-phase process that eliminates the use of volatile solvents and can deposit faster. It is hypothesized that the properties of these membranes will be similar to those that are made via solution-based approaches.

To this end, I have conducted a series of swelling tests to investigate the connectivity of both the solution-based and vapor-based membranes. I employed spectroscopic ellipsometry in conjunction with a liquid cell, where humidity is introduced to the chamber using mass flow controllers that bubble dry Nitrogen through a water container. I then build an optical model that best matches the ellipsometry data in order to extract the film's properties, such as refractive index, surface roughness, and thickness. Since ellipsometry can continuously and quickly measure how the film's thickness responds to changes in humidity, I also hope to extrapolate its diffusion coefficient to better understand how water interacts with these membranes.

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Name: Edward Nusinovich		**Grant Number**	70NANB16H131
Academic Institution: University of Maryland College Park		**Major:** Mathematics - Applied	
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	Pursuing a career in artificial biomechanics and rehabilitation of amputees with trans-tibial and trans-femoral amputations. Planning to go to graduate school in the field.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Science and Engineering Division, Thermodynamics & Kinetics Group		
NIST Research Advisor:	Shengyen Li Carelyn E Campbell		
Title of Talk:	The application of data mining techniques for efficient material design		

Abstract:
For materials that have been in use for an extensive period of time, there is often an established underlying physical model with parameters that account for the behavior of the material. For new materials, the model parameters governing the material properties may not be known. The aim of this research is to automate the process of determining material properties from a limited (and potentially noisy) set of experimental data, and to use this knowledge to help design new materials for specific applications.

A software package was developed that allows a user to input a physical model and an experimental dataset. Based on these inputs the software determines the optimal parameters for the model to best fit the experimental data. Specifically, the software provides the ability to enter a stress-strain dataset, and then determine the tensile and yield stress of the material. Using these inputs, the user can then use a constitutive model for plastic deformation to predict the strain hardening rate of the deformation. The advantage of this approach is that it enables the prediction of the material behavior in both the elastic and plastic regions without extensive material property data and without having to specify the yield stress to determine the behavior.

Another useful feature of the software is its versatility. A user can automatically upload data from a text document, a data file, or an XML schema, without having to transform the files. This significantly reduces the time needed to setup an analysis and provides a powerful way to easily aggregate data from myriad sources.

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Name: Christine Plavchak		**Grant Number**	70NANB16H076
Academic Institution: Washington & Jefferson College		**Major:** Chemistry/Spanish	
Academic Standing (Sept. '16):	Seeking interim employment prior to graduate studies in Fall '17		
Future Plans (School/Career):	Ph.D. in physical or analytical chemistry, and a career in industry or a government facility focusing on NMR spectroscopy		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Science and Engineering Division, Functional Polymers Group		
NIST Research Advisor:	Ryan Nieuwendaal		
Title of Talk:	Determination of ^{1}H NMR spin diffusion coefficients via standard P3HT-PCBM bilayer films		

Abstract:
Bulk heterojunction (BHJ) organic photovoltaics (OPV) are widely studied for their potential use as low-cost solar cells. In the BHJ cell, donor and acceptor organic semiconductor molecules are cast from the same solution to produce an intimately mixed thin film polymer blend. In the BHJ film, intimate mixing (or a small domain size) is needed due to the small exciton diffusion length typical in BHJs. However, this can be difficult to quantify or explicitly measure. ^{1}H combined rotation and multiple pulse spectroscopy (CRAMPS)-based spin diffusion nuclear magnetic resonance (NMR) is capable of measuring 1 nm to 100 nm domain sizes in organic blends and has the required sensitivity for small sample volumes like lab-scale thin films (< 5 mg). One limitation has been the lack of an experimentally verifiable spin diffusion coefficient for calculating the correct domain size via Fick's Laws. In this work, we identified the spin diffusion coefficients (D_{eff}) of poly(3-hexyl thiophene) (P3HT) and phenyl-C61-butyric acid methyl ester (PCBM) by performing ^{1}H spin diffusion NMR on P3HT-PCBM bilayer films of different, known thicknesses. Individual thin films of P3HT and PCBM were fabricated by blade coating onto silicon wafers, which were then formed into model bilayers through a transfer technique with a polydimethylsiloxane (PDMS) elastomer. Spectroscopic ellipsometry and X-ray reflectivity measurements were used to determine bilayer thicknesses.

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Name: Austin Schuberth		**Grant Number**	70NANB16H050
Academic Institution: Kansas State University		**Major:** Mechanical Engineering	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Either attending graduate school or working in industry		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Science and Engineering Division, Mechanical Performance Group		
NIST Research Advisor:	Dilip Banerjee		
Title of Talk:	Finite Element Modeling		

Abstract:

Finite Element Analysis (FEA) is a numerical technique used to approximate solutions to common engineering problems. Engineers often employ FEA to simulate engineering processes under different scenarios, which could have different governing equations (e.g. heat, static equilibrium). This makes it a helpful tool to increase our understanding of the physical world. FEA discretizes a domain of interest into smaller entities called elements and obtains field variables (e.g., displacement, temperatures etc.) at specified points called nodes to approximate the governing equations. In this project, a commercially available software package, Abaqus, was used to conduct FEA of two problems.

The first problem comprises studying the environmental degradation of the U.S.S. Arizona, which is a battleship constructed by the Navy from 1914-1915. The attack on Pearl Harbor left her critically damaged on the front side. Ultimately, she sank and has stayed there under water ever since serving as a symbol and monument of the Second World War. Unfortunately, the corrosive oceanic environment degrades the structural integrity of the ship. As such, the objective of the current FEA work is to predict the longevity of this ship. In order to analyze the ship, a 3-D FEA model, covering an 80-foot midsection, was created using SOLIDWORKS software. Old blueprints and construction photographs provided the dimensions and structure of the ship. The FEA model will ultimately help predict the effects of corrosion and wear from her surroundings to estimate the life of the ship before collapsing.

The second problem involves studying the effects of load reversal in sheet materials used in automotive manufacturing. Researchers are working to develop testing techniques to apply in-plane tension and compression to thin sheets of metal without the occurrence of buckling. FEA is being used to as part of the design process. Baseline experiments were conducted to allow for validation and calibration of the FEA model. The comparison between the model and these experiments are presented in the current work. Once validated, the FEA model will ultimately be used to determine the optimum specimen geometry.

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NIST – Gaithersburg, MD
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Name: Lauren Singer		**Grant Number**	70NANB16H041
Academic Institution: Bucknell University		**Major:** Mechanical Engineering/Physics	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Graduate school for physics and engineering		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Biosystems and Biomaterials Division, Biomaterials Cell Group		
NIST Research Advisor:	Nicholas Schaub Carl Simon		
Title of Talk:	Engineering a Low Cost, Open Source Electrospinning System for Nanofiber Production		

Abstract:

Electrospinning, a process that uses electric charge to produce polymeric nanofibers, is rapidly gaining traction in the scientific community due to its versatility and wide range of applications. Electrospun fibers have a high surface area to volume ratio, high tensile strength, and controllable topography. These properties make electrospun fibers ideal for implementation in tissue engineering, protective clothing, and filtration technology.

The most prominent obstacle to commercialization of electrospinning in fabrication operations is lack of reproducibility. Environmental variables such as temperature and humidity significantly affect fiber diameter and morphology, and equipment that adequately controls these parameters can cost tens of thousands of dollars. The continued advancement of electrospinning technology would be enhanced by an inexpensive and publicly available system for controlling fiber production.

This need was addressed through the development of an open source, easily-modified system for controlled electrospinning and improved process reproducibility. An open source design for a 3D-printable syringe pump was used in a custom-built acrylic glovebox to reduce costs. The environment and electrospinner were controlled through programs written in Python using a simple, open-source computer (Raspberry Pi 3). The program contains a graphical user interface (GUI) that allows the user to track humidity and temperature in the electrospinning environment, control a humidifier to change the humidity, and send commands to the syringe pump. This talk will address the cost, reproducibility, and safety advantages of this open source method of electrospinning, as well as its effectiveness in regulating fiber diameter and fiber surface morphology.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Sarah Smith		**Grant Number**	70NANB16H064
Academic Institution:	University of Kentucky Research Foundation	**Major:**	Chemical and Materials Engineering
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Pursue a graduate degree in chemical engineering focusing in polymer science		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Measurement Science Division, Surface & Trace Chemical Analysis Group		
NIST Research Advisor:	Shin Muramoto		
Title of Talk:	Potential Age Dating of Fingerprints using Time-of-Flight Secondary Ion Mass Spectrometry: Looking at the Diffusion of Fatty Acids on Model Surfaces that Mimic Real World Surfaces		

Abstract:

In forensics, there is enormous value in being able to age date a fingerprint, since the knowledge of the time of its deposition could reveal a suspect's connection to a crime scene, which can at the same time eliminate unrelated suspects and potentially reduce a backlog of evidence waiting to be analyzed. In previous work, the extent of diffusion of fatty acids from the fingerprint onto a surface was used as a marker for determining the age of a fingerprint, using time-of-flight secondary ion mass spectrometry (ToF-SIMS) as an imaging tool. In this subsequent study, the diffusion of palmitic acid was observed on a variety of surfaces for the development of models that can be used to predict its diffusivity and behavior on real world surfaces, accomplished using self-assembled monolayers (SAMs) with (-OH, -COOH, -COOC, -CH3, -NH2, -CF3, -C6H6) terminated alkane thiols that mimic surfaces such as glass (-OH), polyester (-COOCH3), polystyrene (-C6H6), and cooking utensils (-CF3). The polar interface energy of the surfaces ranged from (36.8 ± 1.1) mJ/m^2 to (0.2 ± 0.2) mJ/m^2, which were consistent with energies found on surfaces of commercialized products designed for everyday use. The extent of diffusion of palmitic acid was monitored everyday using ToF-SIMS for 15 days, and the intensity profile of its outward flow was fit to a power model. The diffusivity, determined assuming a semi-infinite plane error-function for mass diffusion, ranged from $(2.1 \pm 1.8) \times 10^{-5}$ mm^2/h on a (-CH3) terminated surface to $(8.3 \pm 2.9) \times 10^{-5}$ mm^2/h on a (-OH) terminated surface, indicating the need to know the properties of the surface for accurate age determination. While the extent of diffusion of palmitic acid was discrete for an average of five days, its extent beyond this time was more difficult to distinguish and more prone to errors, suggesting a need for another marker for measuring the age of older fingerprints.

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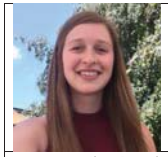
NIST – Gaithersburg, MD
August 2-4, 2016

Name: Karina Stetsyuk		**Grant Number**	70NANB16H136
Academic Institution:	Hood College	**Major:**	Math & Computer Science
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Will attend graduate school to study Environmental Engineering.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Science and Engineering Division, Thermodynamics & Kinetics Group		
NIST Research Advisor:	Lucas Hale Zachary Trautt		
Title of Talk:	Adding automated uncertainty estimates to temperature- and pressure-dependent property calculations of iron from molecular dynamics		

Abstract:

As atomistic simulations become increasingly widespread and easy to do, it becomes even more important for researchers to learn the proper applications of the classical interatomic potentials for optimal, and believable, results. The Interatomic Potentials Repository (IPR) project at the National Institute of Standards and Technology has for years hosted interatomic potentials (force fields) of known provenance, primarily for metallic materials. Now the project is expanding to include an open-source framework to calculate material properties for potentials on the IPR website. This framework can also be downloaded and used outside of the IPR. A number of calculations are being developed in this framework to help users select potentials best suited for their needs, which can include a wide range of applications.

In this study, we focus on measuring lattice parameters of a crystal structure for iron at different temperatures and pressures using molecular dynamics. In order to do this, we implement a method for finding an appropriate section of data in which the structure is at equilibrium. Routines are constructed to properly estimate mean and standard deviation of mean for the lattice parameters and potential energy. We implemented the pymbar method to estimate, via interpolation, properties and their standard deviations at intermediate temperatures and pressures. This improves understanding of potentials and their associated material properties by demonstrating how they behave over a wider range of values than just those explicitly calculated. Results for potentials of pure iron are compared to experimental values. This system serves as a prototype for other elements and alloys and is being integrated into the framework under development.



SURF Student Colloquium

NIST – Gaithersburg, MD
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Name: Kailey Stracka		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland College Park	**Major:**	Materials Science & Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Complete bachelor's degree and pursue graduate school		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Chemical Sciences Division, Chemical Informatics Research Group		
NIST Research Advisor:	Daniel Siderius		
Title of Talk:	Developing a System to Encode Multicomponent Adsorption Isotherms for Standard Reference Data Use		

Abstract:
Adsorbent materials have been used for over a century for important applications including gas purification and separation, water purification, and desiccants. In the past two decades, advances in chemistry have led to the development of new adsorbent materials including activated carbons, silicates, and metal organic frameworks. Because of their high surface areas and selectivity, these new materials can be used to develop more efficient and cost-effective methods to remove pollutants from the air, purify solutions, and catalyze reactions. However, due to the extensive number of ways in which they can be modified such as processing temperature, chemical treatment, and composition, they require a substantial amount of research. Currently, there is poor communication between researchers because they lack standardized experimental procedures, material naming conventions, reference data, and standard formats for data exchange. This has hindered the development of materials capable of solving issues.

A need to improve communication has led NIST to develop a database of Novel and Emerging Adsorbent Materials to aid researchers in accessing and comparing adsorption data. This database is under continuous development and includes only a fraction of the isotherm data that has been published. This summer we helped resolve this issue by digitizing single component isotherms, thereby increasing the reach of the database. Additionally, we expanded the database system to include multicomponent gas adsorption. Multicomponent isotherms are more difficult to digitally encode as the composition of the gas adds constraints that must be recorded to fully describe a multicomponent adsorption experiment. By reviewing several hundred articles on multicomponent adsorption we were able to develop, test, and refine a file format that can robustly and accurately encode this data. This addition is important as it allows for the inclusion of data on selective adsorption of mixtures to represent gases like those found in nature and industry.

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NIST – Gaithersburg, MD
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Name: Sam Underwood		**Grant Number**	70NANB16H057
Academic Institution:	Reed College	**Major:**	Chemistry
Academic Standing (Sept. '16):	University of Oregon, 1st Year Graduate Student		
Future Plans (School/Career):	PhD (Chemistry)		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - ChemBio, Materials Measurement Science Division, Nano Materials Research Group		
NIST Research Advisor:	Justin Gorham		
Title of Talk:	Silver Nanoparticle-embedded Textiles: Preparing and Characterizing a Model System		

Abstract:
Silver nanoparticles (AgNP) exhibit antimicrobial properties and can be embedded into textiles to make clothes, gloves, or bandages with medical utility. AgNP are the most widely commercialized nanomaterial, and rigorous characterization methodologies are therefore necessary to inform consumers and researchers about the properties of these materials. To that end, we have developed methods for preparing AgNP-embedded textiles to use as validation materials, and have used these materials develop characterization protocols for AgNP-loaded textiles using various techniques, including spectroscopy, spectrometry, and microscopy.

Textile silver loading concentration was determined by inductively coupled plasma mass spectrometry (ICP-MS) and X-Ray photoelectron spectroscopy (XPS), specifically examining how homogeneity of loading is impacted by fabric type (cotton vs. nylon) and by aging. Data show that silver loads preferentially on the material's surface (as compared to the bulk) for both cotton and nylon textiles. For cotton, this surface enhancement effect becomes less pronounced as total silver concentration increases, with a surface loading maximum of 5% to 6% silver by mass. Nylon exhibits a higher potential for surface loading of silver, with no maximum concentration found on the range examined. XPS and scanning electron microscopy (SEM) data demonstrate that surface loading occurs in a heterogeneous manner, especially with cotton textiles. Preliminary analysis of SEM images shows that for cotton test materials with intermediate silver concentration, mean AgNP diameter is approximately 40 nm ± 15 nm, with larger diameter for those samples of lower silver concentration. Size distribution for nylon textiles will also be presented, as well as an analysis of how surface silver varies chemically and physically with time.

This study presents rigorous methodologies for determining AgNP size and concentration in a heterogeneous system. As AgNP-loaded products increase in popularity, validation materials and metrology protocols like those developed in this work will become increasingly important.

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Name: Keith P. White		**Grant Number**	70NANB16H053
Academic Institution:	The Pennsylvania State University	**Majors:**	Physics, Engineering Science
Academic Standing (Sept. '16):	Senior Year		
Future Plans (School/Career):	Pursuing an M.S. in Materials Science and Engineering, and potentially a Ph.D. in Condensed Matter Physics.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Science and Engineering Division, Polymers & Complex Fluids Group		
NIST Research Advisor(s):	Jan Obrzut , Yanfei Yang		
Title of Talk:	Engineering of Nano-Carbon Graphene Based Devices & the Effect of Atmospheric Dopants on Graphene's Electronic Properties		

Abstract:

Graphene, a 2-D allotrope of carbon, is best known for its high electron mobility and remarkable tensile strength. Due to the unique physical and electronic properties of graphene, it is of interest in a multiplicity of applications. Being both thin and flexible, as well as transparent, graphene makes for an effective material in flexible displays, compact electronics, and high energy to volume supercapacitors. Due to its organic composition, there is also a means for application in bioelectronics, such as in vivo diagnostic tools, and microbial sensors. Graphene is used as a reference standard of electrical resistance, due to its easily measurable quantized resistance and conductance properties, demonstrated in what is known as the Quantum Hall Effect. Developing an understanding of graphene's interactions with its environment is, therefore, important for both the upkeep of graphene as a reference material and in furthering nanotechnology engineering applications.

In order to quantify effects of exposure to different environments, and circuitry processing chemicals, such as nitric acid vapors, several graphene-based devices have been manufactured for further analysis of the effect of atmospheric dopants on the electrical properties of graphene. The Center for Nanoscale Science and Technology (CNST) allowed for the direct fabrication of graphene test samples, made explicitly for environmental exposure. Among these samples both Hall Bars, and Van der Pauw devices were also created. Fabrication processing was done through a series of e-beam evaporations, reactive ion etches, photolithographic development, and deposition of an epitaxial graphene monolayer. Samples were then analyzed through the application of a non-contact resonant microwave cavity perturbation method. Here, graphene samples are inserted into a waveguide to interrupt the transmission of a microwave signal through a coaxial transmission line. The incident waves are then recorded, along with the reflected and transmitted portions of the wave. From these scattering mechanisms, we determine the complex form of the dielectric constant, as well as the surface conductance of the graphene samples. Analysis of this extracted data allows for the quantification of shifts in graphene's electronic structure caused by atmospheric dopants. Our results indicate that these exposures may introduce either positive charge carriers (p-type) or negative charge carriers (n-type), which adhere to the graphene surface, resulting in notable shifts in surface conductance. Through these experiments, we can better understand graphene's interaction with the environment, especially as to how atmospheric dopants affect the electrical properties of nanocarbon structures. The understanding of these interactions can be applied to help advance manufacturing processes, allow for the manipulation of graphene in aforementioned applications, and will assist in the building of fundamental knowledge necessary for the industrial application of graphene.

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Name: Richard Wu		**Grant Number**	70NANB16H056
Academic Institution:	University of Texas at Dallas	**Major:**	Biochemistry/Healthcare Studies
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	Medical school and/or graduate school		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - MatSci, Materials Science and Engineering Division, Functional Polymers Group		
NIST Research Advisor:	Daniel Sunday		
Title of Talk:	Morphology and Miscibility: Characterizing A-B-A/B'-C Triblock-Diblock Copolymer Blends		

Abstract:

Block copolymer blends are known to self-assemble into a wide range of nanoscale morphologies, such as lamellae, cylinders, and spheres. By adjusting factors such as constituent chemistry, relative molecular weights, and concentrations, the length scales of those morphologies can be tuned for nanopatterning applications. Lamellar structures, in particular, have been extensively investigated for potential uses in next-generation lithography, and lamellae with simple spacing patterns have been produced in directed self-assembly of diblock-homopolymer blends and in triblock-homopolymer blends. However, lamellae with multiple spacings remain difficult to synthesize, and may require alternative blend compositions.

One possible solution could involve triblock-diblock copolymer blends with A-B-A/B'-C compositions (B' comprising the same polymer as B but with different molecular weight). Previous studies on A-B-A triblocks have shown that the lack of a free chain end in the middle B block causes a restricted conformation, which lowers the B block's miscibility, especially with higher molecular weight additives. It is thus hypothesized that in lamellar structures formed from an A-B-A/B'-C triblock-diblock blend with miscible A and C blocks, the triblock A block and the diblock C block will readily mix, but miscibility of the triblock B block and diblock B' block will depend on the relative molecular weights of the B and B' blocks. By fine-tuning the composition of an A-B-A/B'-C triblock-diblock blend with A/C miscibility but B/B' immiscibility, it may be possible to produce novel A-B-A-C lamellar structures with multiple spacings.

The objective of this project is to assess structural morphologies of various triblock-diblock blends with small-angle x-ray scattering testing and MATLAB simulations, and to evaluate the effectiveness of using differential scanning calorimetry to determine triblock-diblock blend miscibility. The triblock-diblock blends were compared with triblock-homopolymer reference blends, and the morphology and miscibility data compiled to create phase diagrams for the triblock-diblock blends and triblock-homopolymer blends.

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Name: Anthony Ayala		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland, College Park	**Major:**	Chemistry
Academic Standing (Sept. '16):	Recent College Graduate		
Future Plans (School/Career):	Pursuing a career in research		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Jacob Tarver, Craig Brown		
Title of Talk:	Selective gas adsorption in metal organic frameworks		

Abstract:
Selective separations of light hydrocarbons are primarily performed by cryogenic distillation, an energetically costly process that could potentially be lowered by the development of solid adsorbents that operate at higher temperatures. Metal organic frameworks (MOFs) represent a promising route for this application. MOFs are made by linking inorganic and organic units, which leads to a high degree of flexibility in the material's geometry, functionality, and pore geometry. MOFs can possess high surface areas, making them ideal candidates for the capture of hydrocarbon gasses. There are strong differences in adsorption selectivity if we change the framework just by using, for example, a different metal and maintaining the overall atomic arrangement of the MOF, or by using a different ligand isomer to make the framework.

Here, we studied the structure and properties of Co_2(*m*-dobdc) (dobdc^{4-}: 2,5-dioxido-1,4-benzenedicarboxylate), and its affinity for hydrogen and several light hydrocarbons. High resolution powder neutron diffraction was applied in order to probe the interactions of the gas molecules with Co_2(*m*-dobdc). Thermal neutrons are highly penetrating, their scattering does not have a strong dependence on atomic number, and are very sensitive to hydrogen/deuterium. Powder diffraction patterns of the MOF, with and without gases, were analyzed using the Rietveld refinement method to determine the atomic scale structure and locations of the molecules. Ultimately, this approach will allow us to rationalize why we observe such different adsorption characteristics for each different MOF and allow the accurate use of theoretic computation methods to get even more detailed understanding of the MOF-adsorbate interactions in order to design ever better suited materials for application.

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Name: Ryan Bonk		**Grant Number**	70NANB16H074
Academic Institution:	Le Moyne College	**Major:**	Physics
Academic Standing (Sept. '16):	Graduate Student		
Future Plans (School/Career):	Attending Syracuse University in pursuit of a Master's Degree in Mechanical Engineering		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research (NIST), Reactor Operations and Engineering Group		
NIST Research Advisor:	Robert Williams and Zeyun Wu		
Title of Talk:	Optimization Study on the Cold Neutron Source for a Proposed LEU Reactor at NIST		

Abstract:
The lifetime of the current NIST reactor (NBSR) will be coming to an end sometime in the middle of this century. A reactor replacement project is underway and currently in the feasibility study stage with the aim of designing a low-enriched uranium reactor featuring a horizontally split core. The NBSR has evolved as a world-class neutron facility and hosts over 2,000 guest researchers annually. Of these researchers, approximately 70% use cold neutrons in their experiments. Cold neutrons are neutrons with energies less than 5 meV and wavelengths greater than 4 Å. They are produced by cold neutron sources (CNS), using moderators that are cryogenically cooled to around 20 K to shift the spectrum of neutrons coming from the core to lower energies.

Preliminary designs of the replacement reactor incorporated a generic CNS design with 20 liters of liquid deuterium. The new reactor design gives us the opportunity to re-design the cold neutron sources to produce the maximum amount of cold neutrons for research. This study attempts to optimize the cold neutron source design using Monte Carlo N-Particle (MCNP) computer simulations. The performance of the cold source was tested using different moderators as well as re-entrant hole geometries in order to find the optimal combination for producing the maximum cold neutron flux. MCNP is also used to calculate the rate of nuclear heat deposition on the new CNS design.

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Name: Ryan Fangmeyer		**Grant Number**	70NANB16H146
Academic Institution:	North Carolina State University	**Major:**	Mechanical Engineering
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	Graduate and pursue a master's degree in mechanical engineering		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Reactor Operations and Engineering Group		
NIST Research Advisor:	Michael Middleton and Bryan Eyers		
Title of Talk:	System Control: Upgraded Refrigerator		

Abstract:

A planned conversion of the NBSR to low enriched uranium will cause a loss of 10% in neutron flux. Compensation for this loss is key to maintaining the NCNR standards of operation, and will partially be achieved by replacing the existing liquid hydrogen cold neutron source with a deuterium cold source. Deuterium is a far more efficient moderator and will significantly reduce the chance of neutrons being absorbed or wasted. The new cold source will require an upgraded 7 kW helium refrigerator, compared to the existing 3.5 kW helium refrigerator. Commissioning of the refrigerator is expected in 2017.

The system control of the new refrigerator consists of HMI programming, extensive wiring, and physical installations. The Programmable Logic Controller (PLC), which contains control logic software, maintains a direct link to the Factory Talk viewer we use to operate all components of the refrigerator. Memory variables that reference instruments, alarms, and display screens were all created for the operation of the HMI aspect of the refrigerator. Wiring diagrams as well as the wiring of each instrument related to the refrigerator must be up to date and accurate. Several controls for the refrigerator were wired, including the turbomolecular pump, various actuators and valves, as well as each PLC connection for the components.

The turbomolecular pump is used for insulation of the cold box of the refrigerator because all of the components within are at cryogenic temperatures. Installation of conduit for the wiring was created to have a permanent pathway for new and existing wires to the power source. Soldering of pins in a terminal box connected to the turbomolecular pump was done to establish a connection to the PLC.

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Name: Daevin Bhathal Hugh		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland, College Park	**Major:**	Mechanical Engineering
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	I plan to complete my B.S. in Mechanical Engineering at the University of Maryland and eventually pursue a Master's Degree in Mechanical Engineering.		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Thomas Gnaupel-Herold, Justin Milner		
Title of Talk:	Characterizing and Verifying Parameters for Two New Mechanical Systems Through the Multiaxial Deformation of Automotive Sheet Metal		

Abstract:
With modern car design's focus on lowering the weight and increasing the safety of cars, the characterizing of the mechanical properties of the multi-axial deformation of various kinds of automotive sheet metal is an important area of research. The main focus of this project was to characterize parameters for future study of two straining devices through the multi-axial deformation of various types and geometries of automotive sheet metal.

To assist in characterizing parameters for these two straining devices, digital image correlation, a method to measure the deformation and strain of a material, was used to obtain data. Though various geometries were tested, they were all subsets of two main geometries; specifically, eight-armed and planar specimens. Eight-armed specimens were deformed using octo-strain, an eight armed device capable of stressing a specimen in eight directions along a single plane, either through tension or compression. Planar specimens were deformed using an in-plane shearing device, a device which uses one clamp to hold the top of a specimen stationary, in tension, or in compression and a second clamp to move the bottom of a specimen in-plane horizontally.

Through many multi-axial deformation tests of both eight-armed and planar specimens, parameters for each device were determined. In addition, the results show that a suitable force control and displacement control loop for both devices have been verified for operation in future tests for uniaxial, equi-biaxial, and strain change paths. Future work includes, testing and verification of control loops for other multi-axial deformations and testing of other metals and geometries; such as, twinning-induced plasticity steel (TWIP) and thicker spot welded specimens of 1010 steel.

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Name: Ian Hunt-Isaak		**Grant Number**	70NANB16H130
Academic Institution:	Oberlin College	**Major:**	Physics
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Pursue a PhD in Physics		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Steven Howell, Joseph Curtis		
Title of Talk:	Small Angle Scattering Calculator for Periodic Boundary Conditions.		

Abstract:
Tools to calculate the small angle scattering of simulated molecular structures are critical to identifying models, which agree with experimental scattering data. Unfortunately, existing calculators are only effective for simulations of dilute molecules, not for dense simulations employing periodic boundary conditions (PBC). A calculator capable of handling PBC would allow for study of scientifically novel and medically applicable systems. Unfortunately no generic calculator for systems with PBC exists, largely because of the difficulty imposed by the finite box. In the parallel field of metallic liquids, efforts have been expended toward understanding and developing the statistical mechanics that allow for intelligent minimization of the effects of the finite size of the simulation box. Drawing from this work, as well as modifying existing calculators to handle simulations of multiple molecules, we have developed software to perform the scattering calculations of interest. A small angle scattering calculator capable of handling dense simulations with PBC will facilitate comparison of molecular simulations to experimental scattering measurements, thereby furthering the study of dense protein solutions that are important in medicine.

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Name: Samantha Isaac		**Grant Number**	70NANB16H158
Academic Institution:	West Virginia University	**Major:**	Physics & Mathematics
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	I plan on attending graduate school and eventually earning a PhD in physics.		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group.		
NIST Research Advisor:	Leland Harriger		
Title of Talk:	Monte-Carlo Exploration of Focused Neutron Guide and Monochromator Geometries		

Abstract:
A new cold neutron source will soon be built at the NIST Center for Neutron Research (NCNR). At this time, the current cold triple axis spectrometer, SPINS, and its neutron guide, NG5, will also be redesigned in order to increase data collection by at least one order of magnitude.

A neutron guide contains surface coatings that line the inner walls which allow the neutrons to bounce down the guide. Currently SPINS is fed by an older generation straight, rectangular guide with Ni58 coating. Newer supermirror guide coatings can greatly increase neutron acceptance, but at a cost of lower reflectivity. Using Monte Carlo simulations, we have explored focusing guide geometries with ballistic transfer of neutrons from source to monochromator.

A second focusing of the neutron beam is accomplished using a double focusing monochromator. Thus, neutron extraction from the moderator is first focused by the guide into a source image and then again, by the monochromator, to the sample position. By including the monochromator into the Monte-Carlo, we are able to fully optimize the flux from source to sample.

After the sample, several cold neutron instruments are under consideration. Two possibilities are the Low Energy Anti-Focusing Spectrometer (LEAF) and the Continuous Angle Multi-Energy Analysis spectrometer (CAMEA). Both spectrometers simultaneously analyze multiple neutron energies over wide scattering angles – something SPINS lacks. Once optimization of the guide and monochromator is complete, similar Monto-Carlo studies will use this front end to compare different back end designs and optimize their performance.

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Name: Richard Leos		**Grant Number**	70NANB16H052
Academic Institution: Texas A&M University - Kingsville		**Major:** Mechanical Engineering	
Academic Standing (Sept. '16):	Graduated		
Future Plans (School/Career):	Pursue a career in the work force and then go to graduate school in the future.		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research (NCNR), Reactor Operations and Engineering Group		
NIST Research Advisor:	Zeyun Wu & Robert Williams		
Title of Talk:	Enhanced Safety Analysis Code Suits for the Reactor Design at NCNR		

Abstract:
A complete safety analysis is imperative for the development and implementation of a nuclear reactor. Part of the new reactor design project at NIST Center for Neutron Research (NCNR) involves intensive thermal-hydraulics based safety analyses. The purpose of this study is to enhance the safety analysis code suites we are currently using by incorporating state-of-the-art critical heat flux correlation into it. There are two goals for the study: (1) Analyze whether or not the reactor will be able to remain within the desired margin of safety for the critical heat flux ratio (CHFR) and onset of flow instability ratio (OFIR), and (2) determine whether the Sudo-Kaminaga correlation (the new correlation) is a viable successor to the Mirshak correlation (the old correlation) in regard to the critical heat flux ratio (CHFR) calculations.

A MATLAB based program will be developed to extract the data from the safety analysis code - PARET/ANL, calculate the CHFR and OFIR values, and analyze the results. Data from several hypothetical design based accident cases will be processed by the program to demonstrate the efficiency and effectiveness of the utility. In doing so, the high probability of safety for the new reactor can be verified.

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Name: Paul Neves		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland, College Park	**Major:**	Physics
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	Pursuing a PhD in Physics		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Nick Butch		
Title of Talk:	Designing an AC Magnetic Susceptometer Measurement Technique in Conjunction with High Pressures and Low Temperatures in Neutron Beam Experiments		

Abstract:
The NIST Center for Neutron Research (NCNR) hosts numerous neutron spectroscopy instruments to measure the structure and dynamics of samples. Alternating current (AC) magnetic susceptometers have proven a valuable tool to probe the magnetic properties of a variety of materials. The ability to perform simultaneous structural and magnetic measurements on a sample at identical high pressure and low temperature conditions would be a valuable addition to NCNR sample environment capabilities. Through the course of this talk, I will highlight key steps taken in the development, construction, and calibration of a new AC susceptometer to operate around this preexisting infrastructure. Then, I will conclude with recently collected measurements demonstrating the efficacy of the new system.

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Name: Madeleine Pasco		**Grant Number**	70NANB16H075
Academic Institution:	Rose-Hulman Institute of Technology	**Major:**	Biology
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Ph.D. in Synthetic Biology or Microbiology		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Antonio Faraone and Erkan Senses		
Title of Talk:	The effect of nanoparticle architecture and softness on the mechanical properties of the composite polymer		

Abstract:
Addition of nanoparticles into a polymer matrix allows for the fine manipulation of the composite material's mechanical properties. While extensive work has been done to characterize the effect of the nanoparticles' shape, size, and concentration on the composite polymer's mechanical properties, the role of nanoparticles' conformation and softness is not fully understood. This study investigates the effects of hard/inorganic and soft/polymeric nanoparticles of similar sizes on the macroscopic flow of the nanocomposites at various concentrations. Rheology was used to measure the viscoelastic properties of the composites, and small-angle neutron scattering was used to investigate the nanoparticle size and dispersion in polymer. With a better understanding of the effect of nanoparticles' architecture and rigidity, polymer nanocomposites can be better optimized for final applications.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Aaron Schankler		**Grant Number**	70NANB16H048
Academic Institution:	Haverford College	**Major:**	Chemistry
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Pursuing an advanced degree in chemistry		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Paul Kienzle		
Title of Talk:	Refining a Markov Chain Monte Carlo Algorithm for Fitting Neutron Reflectometry Data		

Abstract:
Neutron reflectometry is a powerful tool for investigating subsurface interfaces, however we cannot calculate the structure of an interface directly from reflectivity data. Instead, we can build a parameterized model of the structure and adjust it until the calculated reflectivity agrees with the experimental reflectivity. At the NCNR, we use DREAM, a Markov chain Monte Carlo (MCMC) algorithm, which wanders the space of parameters describing the sample structure somewhat randomly, proposing a set of parameters for the model with each step. A candidate set of parameters is either accepted or rejected with a probability based on its agreement with the data. This type of algorithm is more robust to high dimensional, multi-modal search spaces, and when run for enough time, the distribution of accepted points can be used to generate confidence intervals and identify correlated parameters.

The current MCMC implementation has several issues. Most importantly, the fit can occasionally become stuck when dealing with especially complex or unconstrained problems. To determine the proper settings for the fitter and to determine whether a fit is stuck, still converging, or ready to draw conclusions from, users of the fitting program must have some understanding of the underlying fitting algorithm. To address these problems, we have constructed new statistical tests to determine when a fit is stuck and when a fit is converged. We will use these tests to relieve users of some of the tasks associated with fitting a model by making the fitting process more adaptive and less prone to becoming stuck. This will make the fit more robust and easier for non-experts to interpret.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Douglas Scott		**Grant Number**	70NANB16H152
Academic Institution:	University of Delaware	**Major:**	Chemical Engineering
Academic Standing (Sept. '16):	Princeton University, Graduate Student		
Future Plans (School/Career):	After attending graduate school, I hope to conduct research in polymer science within academia or industry.		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Dr. Kathleen Weigandt		
Title of Talk:	Structural and Mechanical Characterization of HPMC/SDS Aggregation through Rheological and Neutron Scattering Measurements		

Abstract:
The incorporation of polymers into commercial surfactant solutions enables control over the consistency and flow properties of many consumer products such as soaps, shampoos, and detergents. However, producers encounter complexity in creating formulations which exhibit desirable consistency due to nonmonotonic changes in solution viscosity as surfactant concentration is varied. This phenomenon results from surfactant aggregation upon polymer chains, yielding proposed nanoscale structures with dimensions suitable for characterization by small angle neutron scattering (SANS). In this study, the structure and rheological behavior of aqueous solutions of highly substituted hydroxypropylmethyl cellulose (HPMC) in the presence of sodium dodecyl sulfate (SDS) was investigated for a wide range of surfactant concentrations. Conductivity measurements were utilized to determine the critical aggregation concentration (cac) and the polymer saturation point (psp) of the system. Subsequent rheological measurements were used to investigate the mechanical properties of solutions with intermediate surfactant concentrations to deduce the impact of aggregation on shear thinning. Static and rheological SANS were then employed to deduce the formation of network, pearl necklace, and micellar structures in addition to relevant size and spacing parameters. With an improved understanding of the interplay between aggregate structure and rheology, producers will be better informed to create products with not only intended functionality but also finely tuned flow properties.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Nathan Super		**Grant Number**	70NANB16H072
Academic Institution:	College of William & Mary	**Major:**	Physics/Computer Science
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Pursing a PhD in Physics		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	William Ratcliff II		
Title of Talk:	BLAND UI: User Friendly Neutron Diffraction Analysis		

Abstract:
Neutron diffraction is a useful tool to analyze the structural properties of a material, which in turn drive the physical properties of that material. While, it is possible to predict how neutrons will scatter from a material with a known crystal structure, the inverse problem of determining crystallographic structure from neutron diffraction measurements is much more difficult due to the loss of phase information. While the traditional Rietveld refinement of diffraction patterns can lead to false solutions, getting stuck in local minima, Bayesian analysis presents a more sophisticated method. At the NIST Center for Neutron Research (NCNR), the program BUMPS (Bayesian Uncertainty Modeling of Parametric Systems), was developed in order to fit problems in complex parameter spaces using a Bayesian methodology. BLAND (Bayesian Library for Analyzing Neutron Diffraction) combines BUMPS with the crystallographic library CrysFML to allow both global fitting of neutron diffraction data, as well as accurate determination of parameters, error bars, and correlations between parameters.

Our work this summer has been focused on creating a more user-friendly interface for BLAND. Whereas previously, users had to write a new source file for each set of data and to interact with BUMPS programmatically, the new interface is a web application that allows the user to enter crystallographic information and observed data and to choose the type of fitting, allowing the server to handle the actual calculations and fits. Future plans include extending the interface to work with magnetic structures, as well as sending feedback to users during long fitting jobs.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Danielle Villa		**Grant Number**	70NANB16H047
Academic Institution: Eastern Washington University		**Major:** Physics and Chemistry	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Pursuing a PhD in Physics		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Qingzhen Huang, Craig Brown		
Title of Talk:	Neutron Scattering studies of the Crystal and Magnetic Structures of Molecular Magnets		

Abstract:
A particular class of molecular magnets consists of magnetic metal centers and organic ligands that can be coordinated together in a variety of ways. Crystal engineering controls these parameters to tailor the material depending on the desired traits. A general interest in molecular magnetism has risen due to these unique properties fueling the research in quantum magnetic phenomena. Antiferromagnets are of particular interest and are characterized by a magnetic exchange interaction (J) between magnetic moments of opposite sign and their tunable single-ion properties (D). Many different techniques, including magnetization and heat capacity, are used to identify and understand these interactions on a macroscopic level. Neutrons, being sensitive to magnetic moments, are an essential tool for measuring down to the single atoms or bonds. Neutron diffraction can identify atom locations as well as the orientation and magnitude of the magnetic moments even in powder samples. Inelastic neutron scattering directly measures the magnetic energy levels, providing determinations of (J) and (D). My research, focused on Ni(II) and Co(II) based molecular magnets, employs the BT-1 Powder Diffractometer for neutron diffraction and the Disk-Chopper Time-of-Flight Spectrometer for inelastic scattering. These experiments are currently in progress.

SURF Student Colloquium

NIST – Gaithersburg, MD
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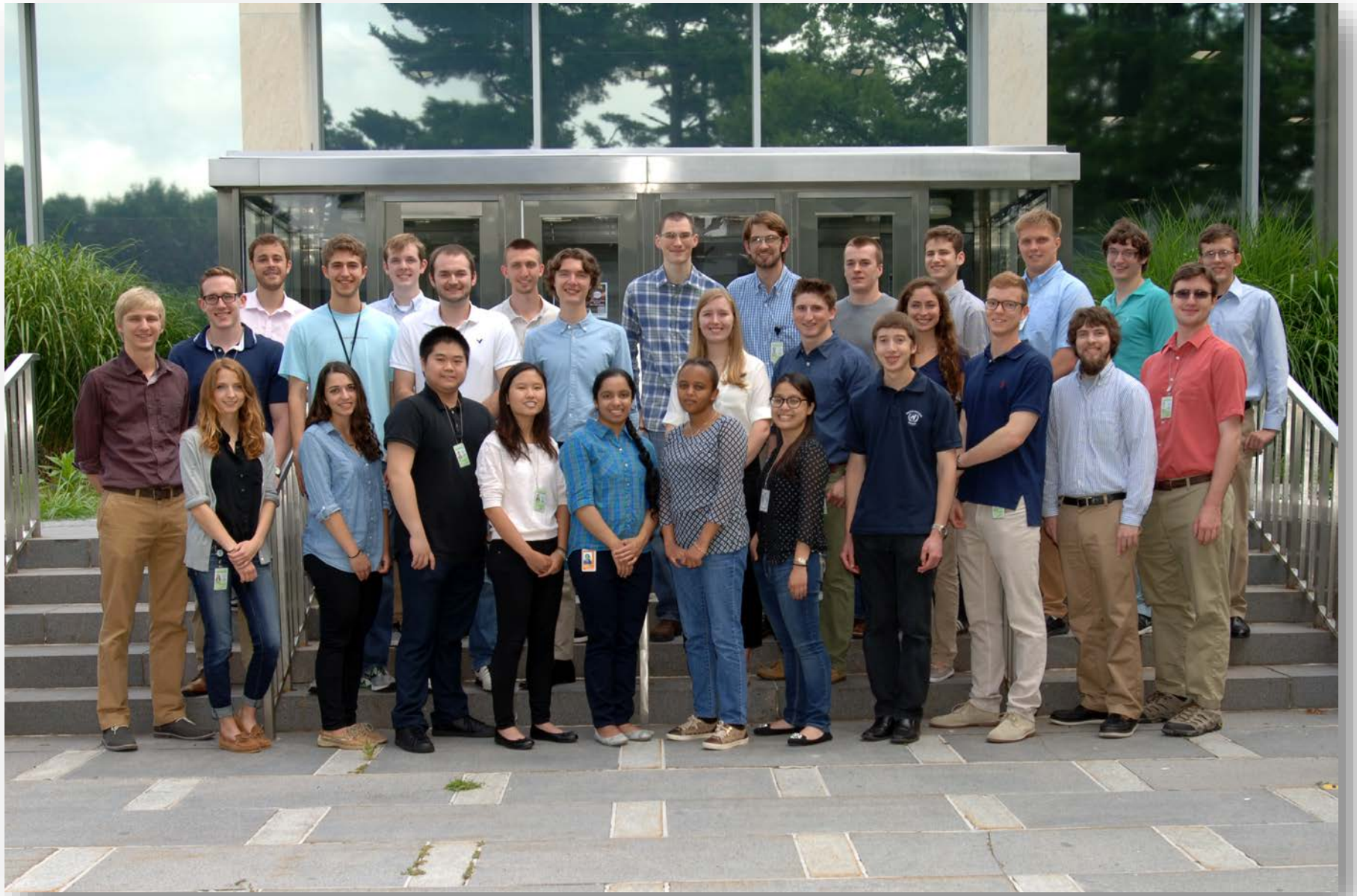
Name: Abdullah Weiss		**Grant Number**	70NANB16H052
Academic Institution: Texas A&M University-Kingsville		**Major:** Mechanical Engineering (Nuclear Engineering Minor)	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Pursue an engineering career in the nuclear industry		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research (NCNR), Reactor Operations and Engineering Group		
NIST Research Advisor:	Bryan Eyers		
Title of Talk:	Compton Suppressed Gamma Spectroscopy of Spent Fuel from NBSR		

Abstract:
The Neutron Beam Split-core Reactor (NBSR) at the NIST Center for Neutron Research (NCNR) operated at a power of 20 MW. Recent studies performed in INL and Penn State suggested that Compton suppressed gamma-ray detection systems can capture more accurate burnup history of the spent fuel. The Compton suppressed instrument improves the accuracy of several analysis algorithms for different radioactive materials by unmasking peaks that are otherwise covered by the Compton continuum. In this project, the primary goal was to successfully measure accurate gamma spectra in order to detect the isotopes that are in the fuel. The obtained data can be used to calculate a burnup by correlating the ^{137}Cs and ^{154}Eu isotopes, and benchmark calculated fuel inventories.

An apparatus was constructed to allow High Purity Germanium (HPGe) and Bismuth Germanate (BGO) detectors to be suspended over the spent fuel pool. A collimator was hung beneath the detectors in order to channel the gamma rays from the fuel to the detectors. The collimator was held at a controlled distance from the fuel element laying at the pool's floor; this was done to avoid over-saturating the detectors by shielding them from gammas using the pool's light-water.

In order to find a safe starting distance between the collimator and the fuel element, a tenth value thickness was calculated using attenuation coefficients that were obtained from recently collected dose rates of four different fuel elements in the pool. Attenuation coefficients were calculated using the dose rates from each fuel element. The average tenth value layer came out to be approximately 1.27 ft. This value is the distance required in the pool's light water to obtain a tenth of the on-contact dose rate for the fuel elements.

The obtained Compton suppressed gamma spectra gave us the integral of power with respect to time for the fuel elements that were measured, which enabled us to compare and contrast them to the burnup history of the NBSR.



PML

Physical Measurement Laboratory (PML)

Electrical Engineering

Buttles, Robert

Chavali, Sai Meghasena

Chiu, Arlene

Davis, Robert

Gamble, Claudia

Goebel, Michael

Guo, Anthony

Gurara, Firehiwot

Liu, Eileen

Montgomery, Karl

Motabar, Lily

Nikolaitchik, Theodore

Phan, Nhi

Rhodes, Corey

Vasilyev, Anton

Verrill, Nathan

Wade, Collin

Zirkle, Theodore

Physics

Barner, Lindsey

Brown, Samuel

Edgerton, Joshua

Graybill, Joshua

Hanson, Joshua

Hastings, Hannah

Lindsay, Maxwell

McClung, Samuel

Paseltiner, Daniel

Riley, Benjamin

Schafer, Benjamin

Townley-Smith, Keeley

Underwood, Samuel

Valdillez, Robert

Walecki, Peter

Ward, Jacob

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Robert Buttles		**Grant Number**	70NANB16H
Academic Institution: University of Maryland College Park		**Major:** Mechanical Engineering/Physics	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Graduate School in some form of physics		
NIST Laboratory, Division, and Group:	Physical Measurement Lab, Sensor Science Division, Thermodynamic Metrology Group		
NIST Research Advisor:	Jacob Ricker, Dr. Jay Hendricks		
Title of Talk:	Automation of an Optical Pressure Standard: Dante's Divine Comedy of Pressure		

Abstract
The Sensor Science division is working to redefine the Pascal in terms of the Boltzmann's constant and helium's refractive index in order to create a new primary method of pressure realization. This device, which has outperformed the current method (mercury manometers), will allow NIST to remove 500 kg of mercury from the lab, drastically reduce the size of the current standards, and be fully automated. Key to this novel technique is the ability to make best in the world pressure measurements that are linked to the index of refraction of a pure gas. To do so, the group has built a device dubbed the "FLOC" or fixed length optical cavity. Because helium's refractivity can be calculated from quantum mechanics, this enables a new and fundamental way to realize pressure. Part of the system involves a differential pressure indicator which cannot reach more than a 1 kPa difference. The current process to move the FLOC to different pressures is time-consuming and prone to error. The solution to this problem is to design a PID (Proportional, Integral, Derivative) control system that follows the FLOC's current pressure while maintaining the 1 kPa difference. With the inclusion of this device, the time consuming process of changing the FLOC's pressure will be automated and take less time to operate. Additionally, the elimination of errors in the control system will reduce the uncertainty of the differential pressure indicator and will therefore allow the highest possible accuracy in the comparison between the FLOC and the mercury manometers.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Sai Meghasena Chavali		**Grant Number**	70NANB16H131
Academic Institution: University of Maryland		**Major:** Electrical Engineering	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	I plan on attending graduate school and earning a Ph.D. in Electrical Engineering		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Radiation Physics Division, Neutron Physics Group		
NIST Research Advisor:	Jeff Nico		
Title of Talk:	Measuring the wavelength of a cold neutron beam for a neutron lifetime experiment		

Abstract:
Measuring the neutron lifetime is an important way to test the standard model of particle physics and provide insight about the early evolution of elements in the cosmos. To improve the precision of the neutron lifetime value and understand systematic uncertainties, we are conducting a new experiment at the NIST Center for Neutron Research (NCNR). Since the neutrons in the beam have varying wavelengths (i.e., energies) and the cross section of the neutron detector is a function of wavelength, one must apply a correction for the wavelength when calculating the neutron beam flux. Error in the calculating the flux results in an error in the value for neutron lifetime. As a result, one must determine the wavelength spectrum in order to decrease this systematic uncertainty. We measured the wavelength spectrum using a beam chopper system and collected the neutron time-of-flight spectra. In my presentation, I will discuss the motivation for this measurement, the method of determining the wavelength, and the results of my measurements.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Arlene Chiu		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland – College Park	**Major:**	Electrical Engineering
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Attending Graduate School		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Fundamental Electrical Measurements Group		
NIST Research Advisor:	Dean Jarrett		
Title of Talk:	Temperature Coefficients on Guarded Hamon Transfer Standards		

Abstract:

Guarded Hamon transfer standards enable 10:1 or 100:1 scaling to high resistances; they are composed of a main resistor network and a guard resistor network. Each individual resistor within the networks is susceptible to drift and thus the entire guarded Hamon transfer standard drifts as well. One variable that causes deviation from predicted drift rate is temperature, which affects the accuracy of measurements but has not been experimentally studied in depth with respect to guarded Hamons. In order to better understand the impact of the individual temperature coefficients of the individual resistors on the guarded Hamon transfer standards the following process was used. Measurements of the main resistor networks of 1 MΩ/step and 100 MΩ/step guarded Hamon transfer standards in series and in parallel configurations were made at 20 °C, 21.5 °C, 23 °C, 24.5 °C and 26 °C in both positive polarity and negative polarity using a high resistance bridge and an automated measurement process with a digital multi meter (DMM), scanner, and reversing switch. The positive and negative polarity measurements were averaged and then corrected against a standard measured at 23 °C ± 50 m°C. Then each individual element in the main resistor networks were measured using the same methods previously mentioned. Measurements of the guard resistor networks and its individual resistor elements were completed in a similar fashion with the exception that no measurements were made using the high resistance bridge for the guard network.

Using the data collected, temperature coefficients of each individual element was calculated and the temperature dependency of each individual resistor was used to generate a simulation of the guarded Hamon transfer standard. The results from the simulation were compared to the actual measured data of the Hamons and different representations for insulation in the LTspice simulation was tested in order to build an accurate model. Having an accurate model will enable resistors of higher nominal value and larger temperature coefficients to be studied and investigated for temperature dependence that may explain variations from the predicted drift rates.

SURF Student Colloquium

NIST – Gaithersburg, MD
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Name: Robert Davis		**Grant Number**	70NANB16H147
Academic Institution:	University of Colorado Boulder	**Major:**	Electrical Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Graduate school for a Ph.D. in electrical engineering, and eventually a career in research		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Quantum Processes and Metrology Group		
NIST Research Advisor:	John Lawall		
Title of Talk:	Broadly Tunable, Narrow Linewidth Lasers		

Abstract:

Modern semiconductor laser technology has progressed rapidly in recent years, and along with it a number of possibilities for their use, both in science as well as industry. However, many of these applications require a stringent characteristic: that the frequency of the laser is highly stable (a very narrow linewidth), and yet can be changed to a desired frequency (broadly tunable). The focus of this project has been to develop a system to achieve those features using a low-cost telecommunications laser primarily controlled via software.

In order to lock the frequency to a steady value, a Fabry-Perot cavity was used, which provides a highly stable reference. Then, using an electro-optic modulator (EOM) and a lock-in amplifier, the frequency could be stabilized for high frequency variations. With this setup, an error signal known as Pound-Drever-Hall could be generated, which could then be used to control the slower changes in frequency via software. Finally, a second EOM can be used to adjust the frequency over the full range. When the complete system is finished, it should allow for a large tunable range for the center frequency (>4 THz), while providing a highly stable (<1 Hz) linewidth.

SURF Student Colloquium

NIST – Gaithersburg, MD
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Name: Claudia Gamble		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland, College Park	**Major:**	Electrical Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Graduate school at some point, but I haven't decided if I want to go right after I graduate or gain work experience first.		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Applied Electrical Metrology Group		
NIST Research Advisor:	Richard Steiner		
Title of Talk:	Testing Smart Watthour Meter Accuracy		

Abstract: As developments are made to transform the electric grid into a "smart grid", new electrical meters are needed. Many are familiar with mechanical watthour meters with rotating disks. They measure energy usage similarly to newer smart meters, but smart meters are built to have greater accuracy and capabilities to communicate with electric companies, allowing each company to better understand energy distribution on the grid. The data transmitted allows more efficient energy allocation and provides knowledge of strains on the electric grid.

Electric power is typically thought to be delivered through sine waves; however, harmonics and distortions are increasingly prevalent in the electric system, and communication signals will be extensive as well. Distorted signals have been previously shown to affect meter accuracy; thus, smart meters must also be tested.

Accuracy tests were conducted on approximately seven electric meters using software to simulate energy consumption. Each meter was tested with sine waves to provide undistorted accuracies and with four different distorted signals, including harmonics modeled after observed signals. The test system measured each meter accurately to 0.04%, and each meter was accurate to 0.2%.

Before testing, we had to understand the software, meters, and test systems. The meters were from multiple manufacturers, so they required different equipment. Some used laser optics for testing, while others used optical couplers to connect to the meter. Occasionally, some meters reported erroneous readings as high as 2000%, possibly due to slight laser misalignments or incorrect test pulses. These were not found to significantly impact our data.

Ultimately, the majority of the smart meters proved able to read distorted signals, as average accuracy results were within the limits of 99.8% and 100.2%. Once harmonics were applied, the mechanical meter had more readings outside the accuracy limits, indicating that smart meters seem better equipped to interpret distorted signals. Time permitting, we intend to test meter accuracy with higher currents, more communication, and different temperatures in order to confirm this in other conditions.

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NIST – Gaithersburg, MD
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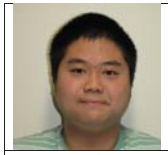
Name: Michael Goebel		**Grant Number**	70NANB16H150
Academic Institution:	State University of New York at Binghamton	**Major:**	Electrical Engineering
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Masters 4+1 at SUNY Binghamton		
NIST Laboratory, Division, and Group:	Physical Measurements Lab, Engineering Physics Division, Nanoscale Metrology Group		
NIST Research Advisor:	Thomas Lebrun		
Title of Talk:	Locking Lasers Using a Digital Servo		

Abstract:

In recent years, usage of laser diodes has increased due to their relatively low price when compared to alternative laser sources. However, these laser sources require high bandwidth controllers to be used effectively. The conventional solution is to use analog control circuits, however given the high performance and niche application of these controllers, they tend to be large and expensive. Custom-built digital controllers have been successfully used to control laser experiments. The core of the setup is a field programmable gate array (FPGA), an array of logical units which can be programmed into different configurations to complete real-time calculations faster than a microprocessor. Though such a device meets the needs of the control system, assembling the required components onto a printed circuit board remains a barrier to replicating these designs.

A more accessible alternative is the Red Pitaya, a general purpose logic board containing all of the required components to interface the FPGA to the laser setup. The board is unique in that it has two high speed analog to digital converters (ADC), and digital to analog converters (DAC). Tests have shown that the hardware operates at frequencies comparable to more highly developed systems previously published. Test results will be discussed that demonstrate the Red Pitaya's effectiveness in locking a laser to optical devices. The success of such tests will be dependent on the optical devices used, but the tests on the controller show that it may meet the technical requirements of many applications while offering a smaller size and lower cost.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Anthony Guo		**Grant Number**	70NANB16H150
Academic Institution:	State University of New York Binghamton	**Major:**	Electrical Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Pursuing an Electrical Engineering career in private industry		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Engineering Physics Division, Nanoelectronics Group		
NIST Research Advisor:	Oleg Kirillov Hyuk-Jae Jang		
Title of Talk:	Metrology for Organic Spintronic Devices		

Abstract:
Spintronics refers to the electronics where information is stored and changed by utilizing electron spins, and is making its way to a multitude of applications such as read heads of hard drives, magnetoresistive random-access memory (MRAM), and magnetic field sensors. The vast majority of devices are made of inorganic materials, but switching to organic-based devices may offer several advantages such as low production cost, light weight, and mechanical flexibility. One of the major effects stemming from spintronics is magnetoresistance (MR). MR is the property of a material or a device to change its electrical resistance due to an applied external magnetic field. There are various types of MR. For example, anisotropic magnetoresistance (AMR) occurs when the angle between the magnetization direction of a material and the direction of electrical current changes.

In organic based systems, different types of magnetoresistance such as organic magnetoresistance (OMR), giant magnetoresistance (GMR), and tunneling magnetoresistance (TMR) can be created and observed. OMR is caused by intrinsic spin-related properties of an organic material. GMR (or TMR) is produced by transport (or tunneling) of spin carriers through an organic material sandwiched between two ferromagnetic electrodes. Developing software programs to acquire data from organic-based spintronic devices is necessary to accurately obtain and analyze spintronic signals such as MR.

We set up electronic instruments to control an electromagnet and a device, and measure its MR effects. A uniform magnetic field is applied to the spintronic device by the electromagnet, and the electrical resistance is measured by a multimeter. The measurements are taken and the instruments are controlled by using a program written with LabView. With this setup, we are able to measure and observe the different types of MR in organic and inorganic spintronic devices.

Progress in the field of organic spintronics is dependent on the development of its metrology. Organic devices tend to have more noise compared to inorganic devices. Obtaining accurate data is crucial to push organic spintronics into more applicable situations in the near future.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Firehiwot Warsa Gurara		**Grant Number**	70NANB16H
Academic Institution:	Montgomery College	**Major:**	Electrical Engineering
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	Pursuing a career in IT and/or doing research in renewable energy		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Engineering Physics Division, CMOS and Novel Devices Group (683.06)		
NIST Research Advisor:	Jason Campbell and Charles Cheung		
Title of Talk:	Magnetic Field Uniformity Through Pole Face Optimization		

Abstract:
Magnets have a wide range of uses in our day to day life. Many of these applications require uniformity of the magnetic field within a volume of interest. For instance, Magnetic Resonance Imaging(MRI) heavily relies on uniform magnetic field formed within a defined geometric region of interest. MRI scanners generate images of body tissues within this geometric region using nuclear magnetic resonance signals generated from the hydrogen atoms of water molecules inside the body. The hydrogen atoms behave like small compass needles which spin randomly. A uniform magnetic field geometric region produces a better alignment of these randomly spinning hydrogen atoms and eventually creates a higher resolution image. Homogeneity is typically achieved by minimizing gap between magnet pole faces and/or using giant magnet pole faces. However, this makes the magnets costly and reduces access to the space between the magnets for doing experiments. Therefore, there is a necessity to reduce the size of the magnet and maximize the pole face gap without losing the uniformity and strength of the magnetic field. The goal of this project is to solve the problem by shaping the pole faces of the magnet.

The project involves both dimension and shape optimization of the pole pieces of a magnet. 2-D COMSOL Multiphysics simulation, Matlab, and Excel have been used to compare uniformities and analyze data. The ultimate goal is to find an optimal shape which has uniformity within a pole face gap of 6cm, uniformity range of 1cm, and a magnetic field strength of 0.3 Tesla(T). Initial 2-D simulations will be converted to more realistic 3-D simulation in order to fully visualize the magnetic field homogeneity. The initial simulations rely on a magnetic field generated by permanent magnets. However, the lessons learned in these simulations also apply to future electromagnet simulations for further control of the magnetic field strength.

The preliminary results we had so far confirmed that adding different sizes and shapes of iron protrusions like triangular, trapezoidal and square shapes at the edges of the pole faces of magnets can greatly improve the uniformity.

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NIST – Gaithersburg, MD
August 2-4, 2016

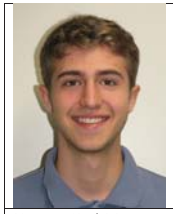
Name: Eileen Liu		**Grant Number**	70NANB16H
Academic Institution:	University of Maryland, College Park	**Major:**	Computer Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Pursuing career in computer or software engineering		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Engineering Physics Division (683), Nanoscale Metrology Group (683.03)		
NIST Research Advisor:	Ravikiran Attota		
Title of Talk:	Using MATLAB in the Development and Optimization of Nanoscale Measurement Techniques		

Abstract:

In recent years, nanoparticles and other nanometer-scale structures have become a heavily researched field of study, with many varied applications in technology and medicine. Although many methods currently exist for the measurement of these structures, such as scanning electron microscopy (SEM) and atomic force microscopy (AFM), many of these methods are prohibitively expensive and require both specialized equipment and time. Conventional optical microscopes are both cheap and readily available, but are limited by the resolution limit, which is established by the wavelength of visible light. However, techniques which allow for optical microscopes to be used in the imaging of nanometer-scale structures are being developed to allow optical microscopes to be used in nanoscale research.

One of these techniques is through-focus scanning optical microscopy (TSOM), which is able to provide three-dimensional information about structures on a nanometer scale. This technique uses a conventional optimal microscope and takes a series of images at various focus points. These images are then used to construct a unique TSOM image which can identify changes in various three-dimensional features. The process of creating TSOM images is not overly complex, but can be computationally intense depending on the size and complexity of images involved. By streamlining the process of TSOM image construction, which involves interpolation, correlation and target matching of several images, the process can be optimized for faster and more accurate TSOM image creation. Various MATLAB optimization techniques are utilized in the process to allow for faster smoothing and image matching of the provided through-focus images.

In addition, experimentation was done into a new technique of more accurately determining nanoparticle sizes, which involves combining scanning electron microscopy (SEM) and atomic force microscopy (AFM) measured top-down projection areas and heights in order to estimate the volume of irregularly shaped nanoparticles. MATLAB was also used to rigorously simulate this technique on randomly generated nanoparticles and determine its accuracy. Both of these techniques improve on existing measurement techniques for nanoscale structures and will allow for a higher throughput and reduction of measurement uncertainty when measuring such three-dimensional structures.



SURF Student Colloquium

NIST – Gaithersburg, MD
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Name: Karl Montgomery		**Grant Number**	70NANB16H
Academic Institution:	University of Maryland	**Major:**	Electrical Engineering
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Going to UMD or another university for grad school. Hopefully I will be going into research as a career.		
NIST Laboratory, Division, and Group:	Physical Measurements Laboratory, Engineering Physics Division, CMOS and Novel Devices Group		
NIST Research Advisor:	Yaw Obeng		
Title of Talk:	Broadband Spectroscopic Characterization of Low-k Dielectric Thin Films for Micro- and Nanoelectronic Applications		

Abstract:

Micro- and nano-electronic devices use different materials of varying dielectric constants for specific applications. The chemistry and physics of these materials play crucial roles in determining the performance and reliability of these electronic devices, especially in low voltages devices. We discuss the use of broadband microwaves (MW) (up to 20 GHz) to characterize hybrid silicon-organic thin films meant for insulation applications. Specifically, we will take advantage of MW propagation characteristics, to extract and examine the relationships between electrical and mechanical properties, and the chemistry of prototypical materials. We use (MW) transmission spectra (S21 amplitude) and FTIR (Fourier Transform Infrared) spectra to detect electrical and chemical changes respectively. Our experiments involve observing the impact of moisture and thermal stress on the (MW) transmission characteristics of selected hybrid silicon-organic thin films. These studies will shed light on the chemical and electrical changes that occur within the dielectric films. These changes could impact the performance and reliability, as well as provide basis for rational selection of organic dielectrics for integrated devices.

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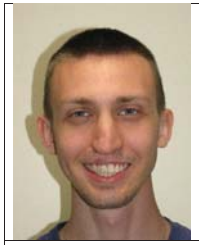
NIST – Gaithersburg, MD
August 2-4, 2016

Name: Lily Motabar		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland College Park	**Major:**	Bioengineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Graduate school for M.S. in Bioengineering		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Engineering Physics Division, Nanoscale Metrology Group		
NIST Research Advisor:	Darwin Reyes-Hernandez		
Title of Talk:	3D Printing Microfluidic Devices with Electronic Functionalities		

Abstract:
The field of microfluidics has matured to the point where the commercialization of devices is expected to increase rapidly. However, a lack in diversity of materials and manufacturing processes restricts the scope and means of low-cost, high-volume production of functionalized microfluidic devices (e.g., biomedical diagnostics). The integration of electronic components is ideal, but complicated by current manufacturing processes due to material adhesion issues and the reliance on post-fabrication modification. Additive manufacturing (e.g., 3D printing) has emerged as a promising candidate for constructing functionalized microfluidic devices. Our aim was to use Fused Deposition Modeling (FDM), the layer-by-layer extrusion of a thermoplastic, as an inexpensive means for 3D printing microfluidics with integrated electronic components. Using a single-extruder 3D printer, we were able to print high impact polystyrene (HIPS) for the microfluidics and fluidic connections, while integrating electronic structures with a conductive poly-lactic acid (cPLA). By maximizing the printing conditions of the conductive polymer, we obtained the minimal resistance range as described by the manufacturer (ca. 150 ohms). To prevent deformation of the microchannel, the device was printed as two parts and solvent-bonded together. The fused device was compliant with standard fluidic connections, water tight, and electrically accessible. Our project demonstrates that mixed-material FDM is capable of fabricating complete microfluidic systems with electronic functionalities.



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Name: Theodore Nikolaitchik		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland, College Park	**Major:**	Electrical Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Attending graduate school		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Engineering Physics Division, Nano Electronics Group		
NIST Research Advisor:	Sujitra Pookpanratana		
Title of Talk:	Molecular Interfaces and its Impact on Electronic Functionality		

Abstract:

In modern commercial electronics, inorganic semiconductors, such as silicon, are used almost exclusively. However, electronics fabricated using organic semiconductors offer several advantages such as lower cost and better mechanical flexibility. Organic materials can also be engineered to have specific electrical properties. By manipulating the materials used in the fabrication of organic field effect transistors (OFETs), it has been demonstrated (Takahashi *et al,* 2006) that the type of transfer characteristics can be controlled by changing the organic metal. Most organic semiconductors display p-type characteristics but these findings confirm the possibility that organic semiconductors can be engineered to a certain functionality. The possibility of being able to control carrier injection in organic electronics increases their viability as an alternative to silicon electronics.

My research seeks to reproduce the electrical results of Takahashi[1] *et al* and physically characterize the interfaces involved in those OFETs. Both the organic metal and organic semiconductor are charge transfer complexes, where a donor (p-type) and acceptor (n-type) molecules are combined and formed in solution. Top contact bottom gate OFETs were fabricated using an organic metal (either tetrathiafulvalene-difluorotetracyanoquinodimethane or tetrathiafulvalene- 7,7,8,8-Tetracyanoquinodimethane) for the source/drain contacts and DBTTF-TCNQ (Dibenzotetrathiafulvalene-7,7,8,8-Tetracyanoquinodimethane) as the semiconductor. Devices were fabricated via vacuum sublimation and deposition onto silicon wafers. Devices were physically characterized using Fourier Transform Infrared Spectroscopy (FTIR) and device behavior was measured using a probe station. From FTIR, we are able to observe shifts in the carbon-nitrogen vibration in DBTTF-TCNQ and TTF-TCNQ/DBTTF-TCNQ samples. Some devices have been measured, but do not display FET behavior. Successful device fabrication has been challenging and is currently ongoing.

Citations
1. APPLIED PHYSICS LETTERS, 88, 2006, 073504

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NIST – Gaithersburg, MD
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Name: Nhi Van Phan		**Grant Number**	70NANB16H162
Academic Institution:	Worcester Polytechnic Institute	**Major:**	Biomedical Engineering
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Pursuing a career in medical imaging and instrumentation within private industry		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Sensor Science Division, Infrared Technology Group		
NIST Research Advisor:	Joseph P. Rice		
Title of Talk:	The Hadamard Transform Hyperspectral Image Projector		

Abstract:
The Hyperspectral Image Projector (HIP) is a spectrally-programmable light source coupled to a spatial projector that is used for a variety of measurements, such as spectral responsivity of optical/infrared sensors or spectral reflectance of materials. The traditional method for measuring spectra is via monochromatic line scanning, which consists of measuring the spectra of individual narrow spectral lines wavelength by wavelength across the spectral range from which data is collected at each wavelength. However, a more efficient algorithm projects a series of spectral lines simultaneously such that wavelengths between the sets are encoded in order that they may be de-convolved using the Hadamard transform to provide the measured spectrum. This method proposes the inherent multiplex advantage offered by the HIP as compared with traditional monochromatic scan. I developed the LabVIEW software for implementing spectral measurements using the Hadamard transform with the HIP. Then I collected spectral measurements to test the performance of the Hadamard technique compared to that of the traditional methods. Analysis of the spectrum produced by the implementation of the Hadamard transform has shown promise in reduction of signal to noise ratio, run time, and hardware use.

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Name: Corey Rhodes		**Grant Number**	70NANB16H
Academic Institution:	West Virginia Wesleyan College	**Major:**	Applied Physics
Academic Standing (Sept. '16):	1st year graduate school		
Future Plans (School/Career):	Pursuing Masters' degree in electrical engineering at Virginia Tech		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Engineering Physics Division, CMOS and Novel Devices Group		
NIST Research Advisor:	Joseph Kopanski		
Title of Talk:	Designing a Charge-Based Capacitance Measurement Circuit for Interfacing with an Atomic Force Microscope		

Abstract:
Measuring the intrinsic properties of devices, such as capacitance, becomes increasingly difficult as the scale of the devices shrink. Knowledge of such properties is critical to ensuring that computer simulations of these devices match closely with real-world operation. In the case of capacitance, traditional measurement techniques become ineffective for nanoscale devices due to the stray capacitance present in the measurement environment. In order to measure the intrinsic capacitance of these nanoscale devices, a charge-based capacitance measurement (CBCM) system is being developed. This system will allow for accurate capacitance measurements down to the femtofarad level, even in the presence of picofarads of stray capacitance. At this stage in the project, the CBCM circuit die has been mounted and wire bonded inside of a SOIC-16 package. Additionally, the differential amplifier present in the circuit has been completely redesigned to employ a true RMS-to-DC converter integrated circuit. This change allows the AC capacitance measurements to be converted to DC signals, which results in a simpler layout and higher accuracy. The final stage of this project will be to layout the CBCM chip and the amplifier circuit on a PCB, and then to interface this system with an atomic force microscope to perform the capacitance measurements.

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Name: Anton Vasilyev		**Grant Number**	70NANB16H
Academic Institution: University of Delaware		**Major:** Electrical Engineering	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Applied Electrical Metrology Group		
NIST Research Advisor:	Jason Underwood		
Title of Talk:	Evaluating Distortion Correction Methods for High-Resolution Digitizers		

Abstract:

High-fidelity conversion of data between analog and digital domains is a critical requirement in industry and defense. Traditionally, the method for characterizing the performance of data converters is to use a calibration instrument with a higher resolution than the device under test. For example, an 8-bit ADC (analog-to-digital converter) could be calibrated with a 16-bit DAC (digital-to-analog converter). While static tests of the data converter's transfer function error are relatively straightforward, dynamic tests are significantly more complicated, as the errors arise from additional nonlinear effects. In my talk, I will discuss my development of two dynamic testing algorithms, their performance with respect to each other and to static testing. I will also show how the algorithms would be used to characterize high-resolution instruments, such as a 24-bit ADC, for which the only pure calibration source is a quantum voltage standard.

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Name: Nathan Verrill		**Grant Number**	70NANB16H098
Academic Institution: Andrews University		**Major:** Electrical & Computer Engineering	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Pursuing a career in engineering-related, international development work.		
NIST Laboratory, Division, and Group:	Physical Measurements Laboratory, Quantum Measurement Division, Applied Electrical Metrology Group		
NIST Research Advisor:	Allen Goldstein		
Title of Talk:	Power System Synchrophasor Data Impairment using Labview		

Abstract:

Modern electrical power transmission and distribution systems are becoming increasingly dependent upon power system synchronized measurement devices such as Phasor Measurement Units (PMUs) for wide area measurement, protection, and control (WAMPAC). PMUs measure power system events and output synchrophasors, which are a windowed estimate of the actual values of power system magnitude, phase, frequency, and rate of change of frequency. Many power system applications consider this synchrophasor data to represent "actual values" on the power system. However, this data is impaired by errors introduced from various sources, including PMU synchrophasor estimation algorithms and network effects. The goal of this project is to create a Labview application that will serve as a framework for testing the effects of impaired measurement data on various WAMPAC applications. This framework uses a module-based, object-oriented programming (OOP) approach to generate both "ideal" and "impaired" synchrophasor data based on a set of customizable parameters and configurations. Once the project is completed, users will be able to generate a wide range of simulated power system events and data impairments in order to test their own application's ability to appropriately handle impaired synchrophasor data.

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Name: Collin Wade		**Grant Number**	70NANB16H
Academic Institution:	Washington University in St. Louis	**Major:**	Electrical Engineering
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Pursuing a PhD in Electrical Engineering		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Engineering Physics Division, Nanoelectronics Group		
NIST Research Advisor:	Dr. Emily Bittle		
Title of Talk:	**The electronic stability of polymer dielectrics for use in low temperature measurements of organic electronics**		

Abstract:
The field of organic electronics has greatly expanded over the past decade to deliver devices that are flexible, inexpensive to fabricate, and promising candidates for biocompatible electronics. Since the method of charge transport within these materials is still not completely understood, designing organic transistors that can be used to create viable electronics is difficult and requires a more profound understanding of the parameters that optimize device functionality. A great deal of the studies performed on organic field effect transistors use silicon dioxide as the substrate and dielectric, though thermal coefficient mismatch between the organic semiconductor and the substrate has been shown to cause drastic changes to charge transport within these devices. The research presented here serves to analyze the electronic stability of polymer dielectrics over a wide range of temperatures and frequencies in the hope that these compounds will be viable for measuring organic transistor behavior at low temperatures. To study these dielectrics, capacitors were produced with various concentrations of Cytop or cross-linked Poly(4-vinylphenol) between aluminum contacts to identify the relative permittivity of these two compounds and how that value changes with input voltage frequency and temperatures ranging from 77-300K. These two compounds were specifically chosen for analysis because their thermal expansion coefficient is more similar to that of monocrystalline organic molecules that have demonstrated band-like charge transport as compared to the more commonly used silicon dioxide. Relatively stable permittivity values have been obtained for a wide frequency range, and we predict that low-temperature measurements will not alter the strength of the dielectric. The results obtained thus far therefore suggest that these two polymer dielectrics will be viable for the fabrication and testing of organic monocrystalline transistors.

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Name: Theodore Zirkle		**Grant Number**	70NANB16H155
Academic Institution:	Walla Walla University	**Major:**	Mechanical Engineering
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Attending a graduate school in order to pursue applied precision engineering		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Engineering Physics Division, Dimensional Metrology Group		
NIST Research Advisor:	Dr. Meghan Shilling		
Title of Talk:	Experiment Design to Analyze the Effect of Roughness and Machining Operations on Light-Based Three-Dimensional Coordinate Measuring Devices		

Abstract:
Light-based, three-dimensional coordinate measuring devices such as articulating arms and fringe projection systems are vital to industry because they can be used to characterize produced parts. However, the effect that different roughness and machining operations have on the measurement quality is unknown. This research project investigated the influence of varying roughness and machining operations on measurement quality.

After initial research, several test configurations were produced and their effectiveness analyzed before a final test protocol was chosen. The protocol's effectiveness was determined by comparing the repeatability of the measurements and the ability of MATLAB to draw meaningful conclusions from the data. A MATLAB script was used to analyze the data, and the standard deviation of the sample, point density returned, and effect of scan direction were all able to be extracted and compared between different surface roughness samples.

Several results have been obtained thus far. For one, the type of machining operation affects values such as the point density returned and standard deviation. Machining operations which produce relatively flat, specular areas have lower returned point densities and higher standard deviations. Additionally, the scan direction has a greater impact on sample measurements which display these qualities when compared to operations which create less specular surfaces. Furthermore, it has been observed that the measurement noise is generally orders of magnitude larger than the surface roughness parameter, Ra.

Overall, the type of machining operation as well as the roughness has an effect on the measurement quality. More research is needed to quantify the characteristics of the machining operations that produce the above results. Ultimately, this research will provide information about measuring various machining types and roughness levels using light-based, three-dimensional coordinate measuring devices

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Name: Lindsey Barner		**Grant Number**	70NANB16H149
Academic Institution: Messiah College		**Major:** Mechanical Engineering	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Pursuing graduate school - Applied Physics		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Division 683, Nanoscale Metrology Group		
NIST Research Advisor:	Andras Vladar and Kate Klein		
Title of Talk:	Machining of Fluidic Structures with Helium Ions		

Abstract:
While helium ion microscopy (HIM) has proven valuable for imaging on the nanometer scale, its excellent resolution coupled with non-negligible mass make substrate sputtering or "machining" capabilities promising as well. When the helium beam is applied to silicon substrates at high doses, however, sputtering (removal) rates of silicon are surpassed by implantation rates, which induce swelling of the substrate surface. When helium implants in the silicon at high doses beyond normal imaging levels ($\geq 10^{17}$ ions/cm^2), bubbles form and eventually coalesce to form large cavities. This causes the silicon to swell, forming an interesting balloon-like protrusion on the surface. With controlled dose patterning, larger and longer cavities can form to make tube-like structures on the silicon surface. Although a considerable amount of research has been done on helium implantation and bubble formation in various substrates, there have been few studies on the bubble coalescence and swelling phenomenon in silicon, which only occurs at very high doses ($\geq 10^{18}$ ions/cm^2). This will be the first effort to thoroughly explore and exploit this phenomenon for the purpose of fabricating silicon "nanopipes." Such a technique could be useful in the design of nanofluidic devices to transport nanoliter volumes of fluids between reservoirs.

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Name: Samuel Brandt		**Grant Number**	70NANB16H154
Academic Institution: Valparaiso University		**Major:** Physics and Humanities	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Undecided		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Physical Measurements Laboratory		
NIST Research Advisor:	Michael Huber, Donald Koetke		
Title of Talk:	Measurement of Schwinger Scattering in Silicon		

Abstract:
The goal of this experiment is to measure the "Schwinger scattering effect" that describes the electromagnetic interaction of a neutron with atomic electric fields. In this experiment we will attempt to measure the rotation of the neutron's spin direction when it undergoes a Bragg scattering from a perfect silicon crystal. On such a scattering or reflection, the neutron magnetic dipole moment (MDM) experiences a torque that rotates it's direction as the neutron passes through the atomic electric field of the silicon crystal. However, the magnitude of the rotation from one such scattering is very small. To amplify the effect, we direct polarized thermal-energy neutrons into a 1 cm wide slot that is cut in a block of pure silicon so as to cause the neutron undergo multiple Bragg reflections down the slot. In this experiment, the Bragg scattering off the opposing walls of the slot produces a change in the orientation of the neutron's magnetic dipole moment that is additative on successive Bragg scatters, thereby producing a measureable change in the neutron polarization over many reflections. When the neutrons emerge from the slot they are filtered by an analyzing supermirror and counted in a neutron detector. The change in the neutron polarization will result in a modified count-rate as compared to neutrons that are not Bragg scattered in the atomic electric field. If successful, this experiment can stand as a proof-of-principle for an alternate method of searching for the neutron's electric dipole moment, a quantity of broad scientific interest and effort.
This summer, we aim to optimize the alignment of the apparatus as well as examine the transport and manipulation of neutron polarization.

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Name: Samuel Hunter Brown		**Grant Number**	70NANB16H144
Academic Institution:	Carleton College	**Major:**	Biology
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Biotechnology		
NIST Laboratory, Division, and Group:	PML, Sensor Science Division, Optical Radiation Group		
NIST Research Advisor:	Maritoni Litorja		
Title of Talk:	Standardizing Firefly Luminescence		

Abstract:

Luminescence is a non-invasive, quantifiable measure used in many bioassays, such as in vivo imaging, cell viability assays, and reporter gene assays. One source of bioluminescence is the firefly enzyme luciferase or chemically altered versions of this enzyme. Luciferase is an effective bioluminescent marker because of its sensitivity, energy efficiency, and simple reagents.

Bioluminescent output is measured in Relative Light Units (RLUs), failing to be on the International System of Units (SI) scale. Luminometers and other instruments to measure luminescence are not correlated with one another, meaning instruments are individually calibrated using their own light source. This makes the RLU an arbitrary unit of measurement, incapable of facilitating measurement comparisons between different instruments due to the inconsistent light standards. The objective here is to have these instruments on a SI scale that ensures reproducibility regardless of the reagent, assay, or wavelength.

Light emitted from a commercial luminometer calibrator was measured using a photodiode, to give the voltage equivalence. Next, a 560nm LED, set to match the typical wavelength of firefly luciferase bioluminescence, was fixed to the same voltage as the commercial luminometer calibrator using a calibration power source. The LED was fashioned into a centrifuge tube with a diffuser, to mimic an ATP assay. The LED was then measured with a luminometer in terms of Relative Light Units (RLU). The RLU measurements were expressed in voltage using the calibrated LED and then converted to watts. This information defined RLUs in terms of watts, a derived SI unit of power. ATP assays at various concentrations were then performed to quantify RLU luminometer readings in terms of watts.

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Name: Joshua Edgerton		**Grant Number**	70NANB16H063
Academic Institution:	Appalachian State University	**Major:**	Physics
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	I plan on going on to graduate school to pursue a career in medical physics		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Division 682, Radiation Physics Group		
NIST Research Advisor:	Denis Bergeron		
Title of Talk:	Quantification of PET Imaging Using NIST-calibrated Radionuclide Sources		

Abstract:
Positron emission tomography (PET), especially paired with computed tomography (CT), is a powerful qualitative technique that can be used to diagnose many diseases, such as cancer and Alzheimer's, and locate areas of interest for treatment. However, PET quantification allows for a wider variety of applications, such as measuring the uptake of fluorodeoxyglucose (FDG) in tumors over an extended period of time to advise treatment. To most accurately measure the biological processes that are the target of PET imaging, the variability and accuracy of the scanner itself must be well known.

To assess the performance of NIST's PET/CT scanner, phantoms containing a homogeneous mixture of water or epoxy and a radionuclide were scanned and compared to the known activity concentration of a master solution. The scans were performed before and after a new calibration of the scanner. The radionuclides used were Ge-68, F-18, and Cu-64. Recovery coefficients were calculated as a ratio of the activity concentration, C_A, measured by PET and the NIST-calibrated C_A to measure the accuracy of the scanner. A better understanding of the calibration protocol and the calibration factors was also developed. It was found that there was a 2.7 % difference between the calculated recovery coefficients between calibrations for the same Ge-68 phantoms, and the last six calibration factors differed by a maximum of 3.4 %. A statistical analysis concluded that the data sets from both calibrations were significantly different. From this data and new knowledge of the calibration protocol, a correction factor may ultimately be derived to return true activity values. Improved quantitation and standardization of PET will facilitate the monitoring of smaller changes in tumor size and disease progression to assess the effectiveness of treatment. In turn, this provides physicians with a more robust basis for diagnosis and treatment planning, leading to more favorable outcomes and saved lives.

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Name: Joshua Reeves Graybill		**Grant Number**	70NANB16H131
Academic Institution:	University of Maryland, College Park	**Major:**	Mechanical Engineering
Academic Standing (Sept. '16):	Graduated spring 2015: BS Mechanical Engineering		
Future Plans (School/Career):	Graduate school		
NIST Laboratory, Division, and Group:	Far Ultraviolet Neutron Detection, Quantum Measurement, Physical Measurement Laboratory		
NIST Research Advisor:	Charles Clark, Michael Coplan, Alan Thompson, Chandra Shahi		
Title of Talk:	Excimer-based Neutron Detection using Far Ultraviolet Noble Gas Emission		

Abstract:

In a noble gas environment, ions liberated from the $^{10}B(n,\alpha)^{7}Li$ reaction, form noble gas excimers (NGE) which have been shown to emit far ultraviolet radiation during radiative decay with 30% efficiency. The product ions ^{7}Li and ^{4}He create thousands of short-lived excimer molecules along their ionization paths lengths, which yield between 5 000 to 15 000 far ultraviolet (FUV) photons per neutron capture. Excimer-based neutron detection (END), therefore, produces an unambiguous neutron signature, proving it a practical design concept for thermal neutron detection. With the current shortage of ^{3}He, an increased incentive for developing alternative neutron detection methods has become paramount. END helps fulfill this incentive by providing many attractive properties compared to conventional ^{3}He detection methods. Among its many attributes, END is affordable, immune to radiation damage, has a large signal gain, and fast response times. These benefits combined with END's unrestricted geometry help to provide a flexible detector platform with robust characteristics.

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Name: Joshua Hanson		**Grant Number**	70NANB16H137
Academic Institution:	Clemson University	**Major:**	Physics and Electrical Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Attending graduate school for Physics.		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Atomic Spectroscopy Group		
NIST Research Advisor:	Dr. Joseph Tan		
Title of Talk:	Capturing Highly Charged Ions in a Radio-Frequency Paul Trap		

Abstract:

Highly charged ions (HCIs) are atoms that have lost all or nearly all of their bound electrons due to high-energy photoionization or collisions with other particles. While HCIs are common in space (e.g., in solar flares, accretion disks, and astrophysical plasmas), the earth consists nearly entirely of neutral matter. The NIST Electron Beam Ion Trap (EBIT) can produce and trap ions with very high charge states using a high current density electron beam concentrated by a pair of superconducting Helmholtz coils. The electron beam ionizes atoms injected into the EBIT by stripping away bound electrons until the ionization energy exceeds the beam energy.

Having control over the motional degrees of freedom of the ions opens up the possibility for precision spectroscopy, including measurements of fundamental constants (such as the fine-structure constant and Rydberg constant) and novel atomic clocks and frequency standards, and the utilization of HCIs for quantum information encoding and processing. The HCIs produced by the NIST EBIT can be slowed to low energy and recaptured by two different types of traps: a radio-frequency Paul trap, which uses a combination of static and oscillating electric fields to confine ions, and a Penning trap, which uses a magnetic field in addition to a static electric field. The combined Penning-Paul ion-capture apparatus enables new methods for manipulating HCIs and measuring atomic properties and quantum processes.

The tandem Penning-Paul trap was modeled using SIMION 8.1, and ion trajectory simulations for Kr^{17+} and Ne^{10+} were performed to determine optimal trapping parameters and understand the ion dynamics within the trap. The results from these simulations were used to generate a number of stability diagrams and figures that describe the motion and dynamics of the ions within the trap for different combinations of trapping parameters. This information can be used in determining the ideal conditions for recapturing HCIs using the experimental setup.

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Name: Hannah Hastings		**Grant Number**	70NANB16H135
Academic Institution: Bryn Mawr College		**Major:** Physics	
Academic Standing (Sept. '16):	Graduate		
Future Plans (School/Career):	Attending University of Pennsylvania's Nanotechnology MSE program starting Fall 2016		
NIST Laboratory, Division, and Group:	PML, Sensor Science Division 685, Optical Radiation Group		
NIST Research Advisor:	Dr. Cameron Miller		
Title of Talk:	Not All AC Power Supplies Are Equal, According to an LED Source		

Abstract:

Solid State Lighting (SSL) products, also known as Light Emitting Diodes (LEDs), have become popular because of benefits they provide such as durability, energy efficiency, and longer lifetimes. As SSL products are now widely used for general lighting purposes, NIST began a Measurement Assurance Program (MAP) in 2010 with support of the Department of Energy to provide proficiency testing for laboratories around the world to make sure that as SSL product use increased, laboratories existed that were capable of measuring these products. MAP 1, the first version of the MAP (another version, MAP 2, began in 2015), consisted of six different lamps and 118 participating laboratories. Measurements of each lamp's total luminous flux, RMS voltage and current, electrical power, luminous efficacy, chromaticity coordinates x and y, correlated color temperature, and color rendering index were taken by NIST, then by the laboratory, and then by NIST again. Last year, the differences between NIST's measurements and the laboratories' measurements for each property were calculated and analyzed along with secondary data about NMI and equipment manufacturers. A major finding of MAP 1 was that laboratories had issues measuring the RMS current of certain SSL products. An experiment was designed to investigate the effect of impedance in the wiring system on the measurements of electrical properties of SSL products.

This Summer NIST focused on collecting data looking at the effect of impedance in the wiring system on measurements of RMS current and voltage, luminous flux, electrical power, and luminous efficacy. The data will be used to improve laboratories' measuring procedure for electrical properties of SSL products to ensure more accurate measurements. We aim to determine a value of inductance and resistance that laboratories can add to their wiring system so that measurements of electrical properties more accurately reflect their values when plugged into a wall outlet.

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Name: Maxwell Lindsay		**Grant Number**	70NANB16H153
Academic Institution: University of Pittsburgh		**Major:** Materials Science and Engineering	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Pursuing a career in materials engineering		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Engineering Physics Division, Nanoelectronics Group		
NIST Research Advisor:	Angela Hight-Walker		
Title of Talk:	Controlled carbon nanotube functionalization for assessing origin of Raman D-band components		

Abstract:

Quantifying defects in single wall carbon nanotubes (SWCNTs) is crucial to understand their fundamental properties and for nanelectronic applications. Raman spectroscopy is a uniquely sensitive optical technique containing spectral features indicative of symmetry-breaking in sp^2 SWCNT carbons, a measure of defects. Intensity growth in the Raman D-band is widely used as an indicator for covalent functionalization of SWCNTs. Surprisingly, despite how limited our SWCNT D-band knowledge is, this information is used extensively in defect characterization. For example, the Raman shift frequency of the D-band in SWCNTs is believed to be dispersive with increasing excitation laser energy, as is seen and well documented in graphene. Yet, early experiments were performed on multi-chirality SWCNT samples, suggesting that the observations reported *could* have been the averaged behavior of the various SWCNT species present.

As chirality separation technology is developing rapidly and single-chirality-enriched samples become more common, it is important to study the chiral-specific D-peak behavior of SWCNTs, including correlating D-band frequency and shape with chirality and (through resonance Raman profile) probing whether or not it really is dispersive. In this study, we investigate the behavior of the Raman D-band in highly-purified (6,5) chiral SWCNTs where defect density is controlled through intentional functionalization with 4-nitrobenzene diazonium tetrafluoroborate. UV-VIS-NIR absorption and photoluminescence are used along with resonance Raman spectroscopy using tunable dye lasers spanning the entire E_{22} absorption window.

Our results show the appearance of a red-shifted, defect-induced photoluminescence peak and an increased D/G intensity ratio in Raman, indicating successful covalent functionalization. Direct comparison of Raman spectra from (6,5) solution before and after functionalization showed significant intensity drop in the Raman graphitic G-peak, suggesting that covalent functionalization on SWCNT sidewalls causes more dramatic effects on the G-peak than on the D-band. Also under investigation is the change in D-band spectral features caused by covalent functionalization.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Samuel McClung		**Grant Number**	70NANB16H102
Academic Institution: Stevens Institute of Technology		**Major:** Physics	
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	I plan to earn a PhD in physics and to become an experimental physicist.		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Sensor Science Division, Fluid Metrology Group		
NIST Research Advisors:	Keith Gillis and John Wright		
Title of Talk:	Unusual Phenomena in Convective and Sonic Gas Flows		

Abstract:

In recent published work, the pressure p and the acoustic resonance frequency f_a of argon gas in a 300 L tank were measured, and the ratio $p/{f_a}^2$ (proportional to the mass M of gas) determined the fractional leak rate $\frac{\frac{dM}{dt}}{M} \approx -24 \times 10^6/hr$ from the tank. The measurements were performed when the tank was exposed to sunshine-driven temperature and pressure fluctuations that were 1000× larger. The reason why the acoustic measurements were insensitive to the temperature profile generated by the asymmetric heating of the tank remains unclear. To study this phenomenon, we developed and calibrated a thermistor probe to measure the temperature profile in pressurized argon gas within the tank when the tank is heated asymmetrically. The measurements provide evidence of convective currents that carry most of the heat between the hot and cool regions, leaving a linear temperature gradient in the bulk of the gas volume. The results of this investigation will help to determine the effectiveness of acoustic methods for flow calibrations and leak detection in large volumes.

In other work, flow through a critical flow venturi was studied to examine the phenomenon of premature unchoking. The standard equation for mass flow, $\dot{m} = C_d C_R^* P_0 A^* \sqrt{M/RT_0}$, is only accurate when the gas velocity is "choked," i.e. when the velocity reaches the speed of sound at the throat. At large ratios between exit and input pressures, the system begins to unchoke. However, researchers have noticed "premature unchoking," which occurs at ratios lower than the threshold predicted by theory. This project hopes to provide clues as to why this occurs. We recorded mass flow as air passed through a venturi at input pressures ranging from 80 kPa to 140 kPa, at which premature unchoking ceased to occur. Results will lead to a better understanding of how premature unchoking depends on input pressure.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Daniel Paseltiner		**Grant Number**	70NANB16H143
Academic Institution: Bates College		**Major:** Physics	
Academic Standing (Sept. '16):	Bates College '16		
Future Plans (School/Career):	Graduate studies in atomic physics		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement, Laser Cooling and Trapping		
NIST Research Advisor:	Ian Spielman		
Title of Talk:	Development of a Digital Holographic Microscope for Imaging Bose-Einstein Condensates		

Abstract:

We present the development of a digital holographic microscope for imaging Bose-Einstein Condensates (BECs). Since their first creation in 1995, atomic BECs have become a powerful tool for experimentally furthering our understanding of quantum mechanics. My teams' work on *in-situ* imaging of one dimensional BECs requires an imaging system with a diffraction limited resolution of 1.0 to 2.0 µm. Achieving true diffraction limited imaging is challenging because of the aberrations and misalignments inherent in any optical system. It has been shown that digital holographic microscopy provides a way to mitigate these imperfections through the digital image reconstruction that it allows. A typical image contains only amplitude information about the field incident on the detector and is generated by a single probe beam that passes through the object of interest. A hologram is formed when an additional reference beam, initially in phase with the probe beam, is recombined with the probe on the detector. This forms an interference pattern from which we extract phase information in addition to the amplitude, allowing the entire field at the image plane to be reconstructed. The field can then be numerically propagated back to the object plane resulting in a digitally reconstructed image. Our image reconstruction process involves filtering of the DC and twin image terms produced by the reconstruction, as well as compensating for aberrations in the system. Finally, this reconstruction technique is implemented in a procedure that simulates absorption imaging of BECs using a test target as the object of interest.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Ben Riley		**Grant Number**	70NANB16H064
Academic Institution:	University of Kentucky	**Major:**	Physics/Mathematics
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	Attend graduate school and pursue a career in physics		
NIST Laboratory, Division, and Group:	Physical Measurements Laboratory, Radiation Physics Division, Radioactivity Group		
NIST Research Advisor:	Dr. Heather Chen-Mayer		
Title of Talk:	An Evaluation of a Dual-Energy Method for CT Imaging		

Abstract:
X-Ray CT scanning is a valuable medical diagnostic tool, allowing for the imaging of internal structures based on the attenuation of photons as they pass through the body. The attenuation of the photons is affected by the composition and density of the scanned materials, in addition to the energy of the incident photons. By conducting scans at different 'energy levels' (different x-ray tube potentials), we can compare the Hounsfield Unit variations of a material from one scan to the next due to spectral dependence. Characterizing this dependence enables us to recover information about the scanned material. In this work, the dual-energy method was used to analyze the composition of several substances, including a whole egg, and other tissue simulating phantoms. By scanning known materials, a machine and energy specific calibration parameter, α_E, was calculated based on the average Hounsfield Unit of the calibration material. This parameter can then be used to back calculate the effective atomic number and electron density of a material, which can give insight into its chemical composition. This was done for a compressible lung phantom, where the effective atomic number of a bronchial substitute was obtained by minimizing the standard deviation of the electron density values determined. The calibrated CT number histogram was then used to calculate the mass of the 'lung' material when the phantom was compressed and uncompressed. This method was also used to analyze the composition of a chicken egg, mainly the shell, white, and the yolk. The method worked well when calculating the electron densities, and found limited success calculating the effective atomic number. It was also found that the quality of data improved significantly when larger energy gaps were used.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: Benjamin Schafer		**Grant Number**	70NANB16H140
Academic Institution:	Hamilton College	**Major:**	Physics and Chemistry
Academic Standing (Sept. '16):	Senior Undergraduate		
Future Plans (School/Career):	Graduate school for either physics or chemistry. Will pursue a career in physics or chemistry in academia or research and development.		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Division 682, aCORN Group		
NIST Research Advisor:	Scott Dewey		
Title of Talk:	Neutron Polarization Measurement on the NG-C Beamline for aCORN		

Abstract:
The aCORN (a CORelation in Neutron decay) experiment measures the angular correlation between the electron-antineutrino and electron following neutron beta decay. The apparatus is currently stationed on the NG-C beamline in the NIST Center for Neutron Research (NCNR). Earlier data taken on the NG-6 beamline suggested a systematic effect due to small residual polarization of the neutron beam. In order to properly account for this effect, the neutron polarization must be determined. This is done by measuring neutron transmission through a polarized ^{3}He spin filter at the end of the beamline. A magnetic field is applied to end of the beamline in order to maintain neutron spin alignment parallel or antiparallel to the ^{3}He polarization as the neutrons approach the spin filter. After passing through a ^{6}Li collimator and fission chamber monitor, the neutrons pass through the spin filter, which is housed in a solenoid in order to maintain the ^{3}He polarization. Transmitted neutrons pass through a second fission chamber. The transmission is calculated by dividing the number of neutrons detected by the downstream fission chamber by that of the upstream fission chamber. Adiabatic fast passage (AFP) is then used to reverse the polarization of the ^{3}He and a second transmission value is calculated. The difference between the two transmission values is used to calculate neutron polarization. Difficulties due to inefficient ^{3}He polarization reversal will be discussed.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: Keeley Irene May Townley-Smith		**Grant Number**	70NANB16H148
Academic Institution: Lamar University		**Major:** Physics/Electrical Engineering	
Academic Standing (Sept. '16):	1st year Graduate Student		
Future Plans (School/Career):	University of Rochester Institute of Optics		
NIST Laboratory, Division, and Group:	Physical Measurements Lab, Quantum Measurements Division, Atomic Spectroscopy Group		
NIST Research Advisor:	Dr. Gillian Nave		
Title of Talk:	Line identification and level analysis of Ti II in the ultraviolet region		

Abstract:
Atomic spectroscopy is the analysis of light emitted from plasmas and is used to determine the chemical composition and the dynamics of the plasma. An on-going project in the Atomic Spectroscopy Group at NIST is to obtain comprehensive spectral data for all neutral and singly ionized iron-group elements (Sc through Ni) and through analysis, obtain more accurate wavelengths and energy level values. The heavy abundance of these elements makes them of interest in astrophysical observations.

The last published study of Ti II in the vacuum ultraviolet region, which ranges from 300-2000 Å, was Huldt et al in 1982. They report wavelength uncertainties of 0.02 Å and have identified 1,240 lines from 1,100-11,000 Å. We obtained better resolved VUV grating spectra from 830 to 3,500 Å at the end of last summer using the 10.7 meter normal incidence spectrograph at NIST and a Ti/Ne hollow cathode lamp, capturing spectra on SWR Kodak photographic plates. Tracks were read with an optical comparator, which has an uncertainty of the position measurement of around 3 mÅ. Based on a similar analysis done for Fe II using the same instrument and methodology, we expect to reduce wavelength uncertainties by an order of magnitude.

At the end of the summer, we aim to have a completed linelist with identified transitions between 1,130-2,900 Å. Ti tracks are calibrated with Pt standards when possible. When unavailable, we use Ti II lines taken from FTS spectra and gas lines from Ne and O for calibration. To help sort through spurious incidences in line identification, we look to Kurucz's calculations of the log(gf) of Ti II and Ti III lines. Another program takes the energy level values of the ion and predicts transitions based on the difference between energy levels. The program can also take observed lines and predict new energy level values. It is our hope to not only identify never before observed transitions but also to identify new energy levels that we could use to break into the lower level region of the atom to aid in the analysis of lines below 1,130 Å. This region is in desperate need of attention but whose analysis is beyond the scope of a summer project.

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August 2-4, 2016

Name: Robert Valdillez		**Grant Number**	70NANB16H146
Academic Institution: North Carolina State University		**Major:** Physics	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	Applying to graduate school for physics.		
NIST Laboratory, Division, and Group:	PML, 682.03, Neutron Physics Group		
NIST Research Advisor:	Hans Pieter Mumm		
Title of Talk:	Measuring the Neutron Spectrum of ^{250}Cf with a Time of Flight Measurement		

Abstract:
The neutron spectrum of ^{252}Cf is well known because Cf neutron sources are made with a large percentage of ^{252}Cf and a small percentage of ^{250}Cf. The half-life of ^{250}Cf is 13 years. In comparison, the half-life of ^{252}Cf is only 2.6 years. ^{252}Cf decays into ^{248}Cm which has a very long half-life of 340,000 years. As a result of the different decay rates, old Cf sources now contain a higher percentage of ^{250}Cf. Determining the neutron spectrum of ^{250}Cf is necessary because instrument calibration is done using these old ^{252}Cf sources under the assumption that the neutron spectrum of ^{250}Cf is the same as ^{252}Cf. Our experiment will test the validity of this assumption and provide the necessary information to be used in precision device calibrations performed in the future. We measure the neutron spectrum using a time-of-flight technique. The measurement works by determining the time difference (and thus neutron energy) between prompt gamma rays detected in a NaI crystal detector and neutrons detected in an organic liquid scintillator detector placed 2.61 m apart. Backgrounds were accounted for by taking two sets of data; one set was taken with a shadow cone and the other was taken without. The shadow cone was placed between the source and the neutron detector directly in front of the source. The shadow cone deflected neutrons that were traveling in a direct line toward the neutron detector. Subtracting data taken with a shadow cone from data taken without a shadow cone eliminates background data. In my presentation, I will discuss the uncertainties in the measurement, experimental set up, data acquisition, data analysis, and results.

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August 2-4, 2016

Name: Peter Walecki		**Grant Number**	70NANB16H138
Academic Institution:	Florida Atlantic University	**Major:**	Electrical Engineering
Academic Standing (Sept. '16):	First year of Graduate School		
Future Plans (School/Career):	Brown University Graduate School		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Radiation Physics Division, Dosimetry Group		
NIST Research Advisor:	Dr. Ronald Tosh		
Title of Talk:	Radiation Dose Metrology through Water Calorimetry		

Abstract:
In the medical field, it is important to know and control the precise amount of radiation dose that a patient receives during various procedures. This talk covers research into potential ways in which current radiation standards can be updated in order to expand the scope and improve the accuracy of existing metrology schemes.

The main technique to be discussed is water calorimetry through interferometry, in which an interferometer is used to monitor changes in the index of refraction caused by temperature increases due to an absorbed radiation dose. Several methods for simulating such temperature increases are presented, including sample rotation, Peltier heater/coolers, as well as actual X-Ray radiation. These methods were then tested by using a Mach-Zehnder Interferometer setup, in which one of the beams is passed through the water to be tested. The resulting fringe phase shifts in the interferogram was then extracted and analyzed in order to determine the relationship between phase shift and temperature change.

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NIST – Gaithersburg, MD
August 2-4, 2016

Name: Jacob Wolfgang Ward		**Grant Number**	70NANB16H079
Academic Institution:	Arizona State University	**Major:**	Physics and Computer Science
Academic Standing (Sept. '16):	1st Year Graduate School		
Future Plans (School/Career):	Graduate school at UMD in chemical physics		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurements Division, Atomic Spectroscopy Group		
NIST Research Advisor:	Dr. Gillian Nave		
Title of Talk:	Energy Level Optimization of Quadruply Ionized Nickel (Ni V)		

Abstract:
Quality spectroscopic measurements that elucidate atomic features such as wavelengths, energy levels, and oscillator strengths are of critical importance to many disciplines in astrophysics. The NIST Atomic Spectroscopy Group provides the astronomy community with the most modern and accurate atomic reference data possible in order to support the wide array of astronomy projects supported by institutions such as NASA. In particular, the iron group elements (chromium through nickel) have been highly useful to the astronomy community, but have serious deficiencies in regards to their available reference data.

As a part of a larger project to improve the atomic reference data for the iron group elements, I will discuss my work with quadruply ionized nickel (Ni V), which was last studied in 1975. The focus of the discussion will be on the use of an energy level optimization program (LOPT) and its applications for Ni V. One of the results of the Ni V energy level scheme produced by LOPT is a set of Ritz wavelengths (derived from energy levels) that often have lower uncertainties than the corresponding measured wavelengths.
In order to fully discuss the behavior and efficacy of LOPT with Ni V, I will also provide a brief presentation and comparison of the measured Ni V wavelengths and intensities I have worked on during my previous two summers at NIST to those found through LOPT. Ultimately, I will demonstrate the improvements in atomic reference data that are possible with the facilities available at NIST.

SP

Special Programs

Ekwuru, Miriam

Emelike, Joseph

Gilpin, Anna

Resnick, Benjamin

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2016

Name: Miriam Ekwuru		**Grant Number**	70NANB16H
Academic Institution: Coppin State University		**Major:** Biology	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	After my undergrad, I plan on joining the Air Force		
NIST Laboratory, Division, and Group:	Technology Partnership Office/ Special Program		
NIST Research Advisor:	Paul Zielinski		
Title of Talk:	Commercialization of Inventions in the fields of Bio-manufacturing and Medical Devices		

Abstract:

Technology Transfer is a foundational part of the commercialization of new technology. It is more than simply the transfer of documents; it deals with all aspects of the transfer of knowledge and technology to the commercial manufacturing unit to guarantee consistent, safe, and high-quality product. The Technology Partnerships Office is responsible for gathering information on inventions emerging from research conducted at NIST. When inventions occur at NIST, the inventions are then reviewed in order to decide whether or not filling a patent application will aid in commercialization. My project was to review and collect relevant information about inventions in the bio-manufacturing and medical devices sector that have resulted from NIST research. I developed a set of categories that grouped the technologies into related technology areas and summarized each invention. I wrote invention summaries in that translated complex scientific and legal language into terms that communicate the value of the invention in order to market the technologies to potential licensees. Creating these summaries required me to interview the inventors to get better understanding of the invention and its potential applications. I then complied into brochure for marketing purposes that will be used at biology related technology events and prepared a summary review article on the state of NIST work in this sector.

In addition, I worked with Minority Business Development Agency (MBDA) to enable a nation-wide discussion between federal laboratories and MBDA Centers. This work entailed a review and categorization of thousands of MBDA customers into industrial and technology sectors. This information will later be aligned with technology data from across the federal laboratory network to better link the available research capacity of the labs with the business clients of the various MBDA Centers.

SURF Student Colloquium

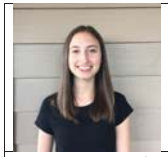
NIST – Gaithersburg, MD

August 2-4, 2016

Name: Joseph Emelike		**Grant Number**	70NANB16H
Academic Institution: Bowie State University		**Major:** Computer Science	
Academic Standing (Sept. '16):	Senior		
Future Plans (School/Career):	I am pursuing a career as a software engineer with a focus on machine learning software.		
NIST Laboratory, Division, and Group:	Special Programs		
NIST Research Advisor:	Reva Schwartz		
Title of Talk:	Golden Cross Section		

Abstract:

Speaker recognition is a subfield of human language technology that focuses on identifying who is speaking. Forensic science is interested in speaker recognition because it often occurs as evidence in criminal investigations when there is no other lead. Improving speaker recognition is important because it can provide a more reliable source of evidence in criminal cases that are centered on, or supplemented by, audio recordings. The ability to identify an individual based on an audio sample is currently a difficult task to perform for machines and humans alike, because of the variable nature of the audio quality, speaker's voice, or both. Even in everyday conversations the speaker's mood or state of health can significantly impact how they speak. Also there is great variability in recording quality due to noise, recording conditions, or working condition of the recording equipment. For our study we will focus on determining where machines outperform human evaluators in identifying speakers. In order to accomplish our goal there will be two initial phases of listener testing. To collect data from naïve listeners, as well as professional listeners, a website will be developed that will allow for the survey to be taken and the responses will be recorded in a database. For the machines, we will do an all models against all files comparison which will output a score for each trial. The results will then be compared with the responses given by the human examiners. Both the machine trials and the human trials will be of paired audio files from the same data set. The portion of the data set we used consists of audio samples from 74 males with varying emotion and content. The machine results have been successfully collected and the human results will be collected over an extended time period.



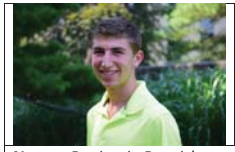
SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Anna L. Gilpin		**Grant Number**	70NANB16H158
Academic Institution:	West Virginia University	**Major:**	Biomedical Engineering
Academic Standing (Sept. '16):	Junior		
Future Plans (School/Career):	Graduate school followed by a career in research & development of biomaterials		
NIST Laboratory, Division, and Group:	Laboratory Programs, Standards Coordination Office HQ (SCO) in Conjunction with Material Measurements Laboratory (MML) Biosystems and Biomaterials		
NIST Research Advisor:	Clare Allocca, SCO and Sumona Sarkar, MML		
Title of Talk:	What is the Meaning of Life?: Terminology and Measurement Assurance for Biotechnology Standards		

Abstract:

Biotechnology utilizes biological processes to create technologies that improve public health and encompasses a wide range of areas including cell and gene therapies and drug development. Recent innovation has led it to become one of the world's most profitable and influential industries. The International Organization for Standardization (ISO) has formed Technical Committee (TC) 276 to create standards specific to this industry and to optimize the development and production of biotechnology products. ISO Standards have achieved consensus across international experts and are underpinned by high-quality measurements and processes. My work has supported two key aspects of standards development for ISO/TC 276: terminology and analytical methods. Clear and mutually understood definitions are critical to measurement assurance. In this work, terms were collected from current TC 276 working drafts on topics including cell counting, cell characterization, and nucleic acid quantification and aggregated into a Terminology Compendium. Terms were also extensively searched to identify definitions within reputed sources (i.e. existing standards, journal articles, and medical dictionaries) to serve as a resource for TC 276 working group experts. Standards to address analytical methods are based on validated and robust methods supported by measurement assurance. This work focused on improving the confidence of cell viability measurements, a key aspect in cell counting and characterization standards. Using design-of-experiment strategies, we evaluated image analysis parameters used by automated counters to generate cell viability data. Results demonstrate that viability analysis is sensitive to these parameters and specific settings may not be robust to all types of cell conditions that could potentially be found in a biotechnology process. As a consequence, appropriate strategies are suggested for establishing image analysis parameters to improve confidence in image-based cell viability analysis.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2016

Name: Benjamin Resnick		**Grant Number**	
Academic Institution:	Case Western Reserve University	**Major:**	Mechanical Engineering
Academic Standing (Sept. '16):	Sophomore		
Future Plans (School/Career):	Graduate and enter industry		
NIST Laboratory, Division, and Group:	Special Programs, Technology Transfer, Technology Partnership Office		
NIST Research Advisor:	Paul Zielinski		
Title of Talk:	Marketing and Licensing of Microscopy Technology		

Abstract:

Every day, NIST scientists are working hard to advance measurement science, standards, and technology in a meaningful way. While this technology can be very beneficial to the American people, it is often difficult to provide the public access to this technology. It is critical that the American people can reap the benefits of the hard work of the NIST scientist.

One way NIST is able to get the technology they develop to industry is by licensing the technology to the private sector and allowing them to incorporate the NIST's inventions with their products. To assist in the marketing and licensing of NIST technology, I developed summary material on NIST work in the field of microscopy. I reviewed patents, presentations, and other documents pertaining to the field of microscopy and the NIST inventions in order to group and describe the inventions in a meaningful way. I described subareas related to microscopy, such as electron microscopy and atomic force microscopy, and categorized the NIST inventions that were related to each subarea. I developed a brief description of each invention translated the complex scientific and legal language used into a business description. I met scientists across NIST to validate my work and gain a greater understanding of the field. Ultimately, the goal is for company's around the country to license the microscopy technology the scientists here at NIST have developed. The work was used as a basis for a NIST display at the Microscopy and Microanalysis 2016 Conference in Columbus, Ohio.

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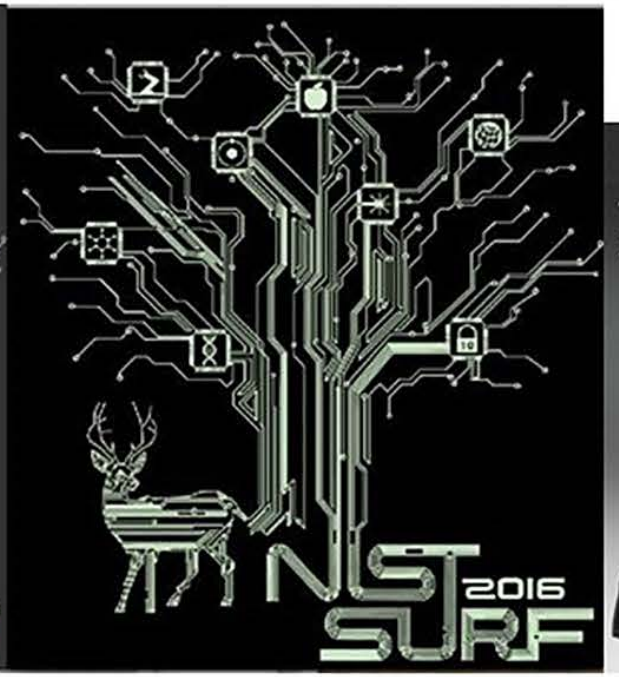
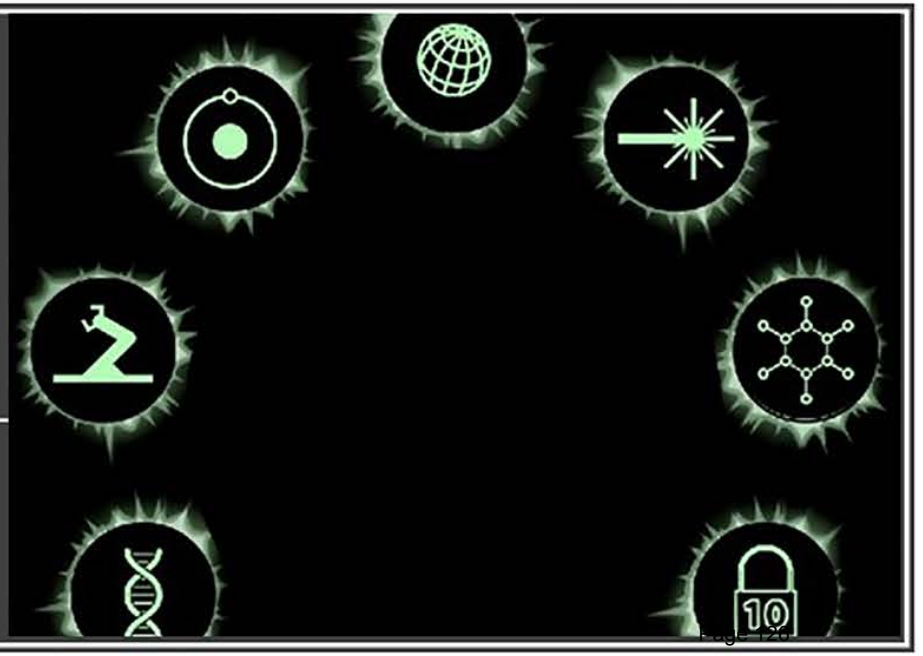
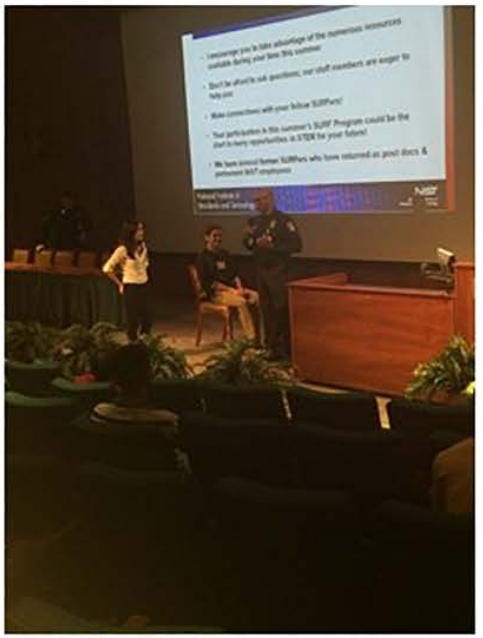
2016



SURF
T-Shirt
Designs






Introduction to NIST
Health Unit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2016

SURF STUDENTS BY ORGANIZATIONAL UNIT

OU	Last Name	First Name	Mentor	University	Title of Talk
CNST	Sloan	Arthur	Liya Yu	Auburn University	Self-Aligned Double Patterning as a Technique to Improve the Critical Dimension of i-Line projection lithography
CNST	Beck	Gillenhaal	Vladimir Aksyuk	Washington and Lee University	Modeling of surface plasmon polariton coupling on a periodic grating and electro-optic polymer for faster spatial light modulation
CNST	Wong	Gina	Robert McMichael	University of Maryland - College Park	Controlling a nitrogen-vacancy center diamond to measure magnetic properties at the nanoscale
CNST	Scaletta	John	Amit Agrawal	Williams College	High-Q Surface Plasmon Resonator for Terahertz Time-Domain Spectroscopy
CNST	Watson	Martha	Lei Chien	George Washington University	Fabrication of Nano-scale High-Aspect-Ratio Structures through a Newly Devised Etching Process
EL	Springer	Adam	Justin Whiting	Northern IL University	Dynamic Characteristics of the Recoater Arm used in the Direct Metal Laser Sintering Process instead of Dynamic Characteristics of the Recoater Arm used in the Powder Bed Fusion Process
EL	Stoddard	Alexander	Doug Thomas	Davidson College	Squareness - Numerical Errors in The Utilization of Machine Tools for Engineering Processes
EL	Nellis	April	Peter Denno	University Maryland College Park	Verifying Analyses of Manufacturing Processes Using Predictive Models and Ontologies
EL	Kifle	Behailu	Paul Stutzman	University District Columbia	Phase Analysis of Portland Cement Clinker by Scanning Electron Microscopy and X-Ray Powder Diffraction
EL	Haile	Bruk	Kathy Butler	University District Columbia	Developing a database using GIS for extreme fire behavior
EL	Krueger	Christina	Jarred Heigel	University Maryland College Park	Seeing between the Lines: Layerwise Imaging for Metal Additive Manufacturing
EL	Kamieniecki	Daniel	Scott Jones	Stevens Institute of Technology	3D Printing Cement: Charactarization of Printable Cement Pastes
EL	Hanson	Edward	Jennifer Helgeson	University Maryland Baltimore County	Community Resilience: Measuring Economic Benefits of Planning for Natural and Manmade Hazards
EL	Auth	Eric	Rik Johnsson	University Maryland College Park	Wind and Separation Distance Effects on Fence Fire Spread in the Wildland Urban Interface
EL	Goh	Justin	Karl Van Wyk	University Maryland College Park	Simulation Assisted Robot Hand and Arm Programming for Planning and Simplifying User Experience
EL	Wakeman	Katrina	Erica Kuligowski	American University	Alterting the Public in Community-wide Disasters: A Literature Review on Outdoor Warning Sirens
EL	De Jesus Morales	Kenneth	Mauro Zammarano	University of Puerto Rico	Towards a Robust Bench-scale Test for Predicting Smoldering Ignition of Residential Upholstered Furniture (RUF)
EL	Li	Kevin	William Bernstein	University Maryland College Park	Defining a Similarity Metric for Manufacturing Processes
EL	Rebrov	Kirill	Randy McDermott	University Texas Austin	A Correction for Velocity Penetration Error at Immersed Boundaries in the Fire Dynamics Simulator (FDS)
EL	Yeh	Malachi	Eric O'Rear	University Maryland Baltimore County	BIRDS: Quantifying Sustainability in Commercial Buildings
EL	Mennu	Matlock	Greg Vogl	University South Florida	Sensor-Based Diagnostics of CNC Linear Axes
EL	Parsons	Matthew	Ferraris/White	Purdue University	Quantitive Analysis of Cement Paste Performance via Oscillatory Rheology
EL	Han	Muhong	Mauro Zammarano/Shona li Nazare	East Carolina University	Fire-Blocking Performance of Laminated Barrier Fabrics
EL	Peterman	Nathan	Paul Witherell	Purdue University	Creating Design Allowables for Additively Manufactured Parts
EL	Aboul-Enein	Omar	Roger Bostelman	Salisbury University	Augmented Reality Marker Tracking for Multi-Robot Registration
EL	Seiler	Patrick	Tim Zimmerman	Texas Engineering Experiment Station	Assessing the Impact of Cybersecurity on Networked Control Systems
EL	Hoddinott	Philip	Glen Glaeser/Amanda Pertzborn	Rensselaer Polytech Inst	Design and Construction of Intelligent Building Agent Laboratory
EL	McIntrye	Rachel	Behrang Hamadani/Brian Dougherty	University Maryland College Park	Temperature Dependent Measurements of Photovoltaic Solar Cells
EL	Youssef	Raef	Gordon Shao	University Maryland Baltimore County	Implementing the ISO 15746 Standard and the Optimization Metamodel for Process Parameter Optimization
EL	Leader	Robert	Natascha Milesi-Ferretti	Arizona State University	Tools for the Ongoing Commissioning of Buildings
EL	Weaver	Samantha	Xiaohong Gu	University Maryland College Park	Impacts of Temperature, Relative Humidity, and UV Source on EVA Degradation in Accerated Weathering Tests
EL	White	Shawn	Brandon Lane	Arizona State University	Dynamic and Mechanical Properties of Metal Powder
EL	Caren	Stephen	Li Piin Sung	Wayne State University	Artificial Sunny Days: Impact of Temperature on Polyethylene Photodegradation Under Accelerated Weathering
EL	Siddiqui	Tawsif	Yan Lu	University Maryland College Park	Schema and Ontology Development for the Additive Manufacturing (AM) Database
EL	Johnson	Theodore	Nicholas Dagalakis	Georgia Institute of Technolgy	Control System Implementation for Motorized Dynamic Bending and Calibration Machine
EL	Winnard	Thomas	Greg Vogl	Andrews University	CNC Linear Axis Diagnostics via Sensors
EL	Varma	Vaughn	Yan Lu	Rochester Institute of Tech	The Internet of Things on the Shop Floor: Design and Implementation of a Service-Oriented Architecture in Manufacturing Systems Utilizing B-SCADA's Status Enterprise
ITL/CLT	Addo	Derrick	Ya-Shian Li-Baboud	Bowie State University	Synchronizing Video Playback on a Tiled Display Wall
ITL/CLT	Aliakbar	Soheil	John Libert/Mary Theofanos	Towson University	Can't Touch This: Usability of Contactless Fingerprint Acquisition Devices

OU	Last Name	First Name	Mentor	University	Title of Talk
ITL/CLT	Collazo-Martis	Ramon	Apostol Vassilev	University of Puerto Rico	Strong Key Generation on Conventional Computer Systems Enabled by a Remote Entropy Source
ITL/CLT	Cooper	Samuel	Stephen Langer	Fayetteville State University	Detecting malicious users and compromised accounts using user behavioral models for the C-Force Enterprise's cloud service
ITL/CLT	Dare	Christopher	Larry Bassham	Virginia Polytechnic Institute and State University	Latency of Lightweight Cryptographic Algorithms
ITL/CLT	Dash	Aditya	Lotfi Benmohamed/Abdella Battou	University Maryland College Park	Performance Monitoring and Instrumentation of Named-Data Networks
ITL/CLT	Davila	Ian	Doug Montgomery	University of Puerto Rico	Test and Measurement of Software Defined Virtual Networks
ITL/CLT	de la Vega	Jose	Doug Montgomery	University of Puerto Rico	Test and Evaluation of Network Anomaly Detection Technologies
ITL/CLT	Deng	Myra	Isabel Beichl	Columbia University	A Probabilistic Method for Counting the Number of Linear Extensions in a Partially Ordered Set
ITL/CLT	Dougherty	Eric	Sandy Ressler	Millersville University of Pennsylvania	Virtual Reality on the World Wide Web
ITL/CLT	Dunkers	Dan	Judy Terrill	Drexel University	Using the CIE-LAB color space to improve the analysis of tests across system differences for the CAVE (Computer Assisted Virtual Environment)
ITL/CLT	Fulton	Kelsey	David Waltermire/Lee Badger/Dmitry Cousin	Millersville University of Pennsylvania	Unwinding the Runtime Stack: Application Runtime Analysis for Anomaly Detection Research
ITL/CLT	Henrich	Janelle	Martin Herman	American University	Finding the Matching Pair: The Use of Graph Theory in Forensic Footwear Analysis
ITL/CLT	Hockley	Stephen	Michaela Iorga/Martin Herman	Shepherd University	Building a Cloud Forensic Reference Architecture: Leveraging AWS CloudTrail to Identify Forensics Artifacts.
ITL/CLT	Indictor	David	Timothy Hall	SUNY Binghamton	Machine Learning for Spectrum Prediction
ITL/CLT	James	Bruce	Alden Dima	University Maryland Baltimore County	Out of Time: Abstracting Temporal Constraints from Time-Based Data in Non-relational Databases
ITL/CLT	Kasner	Jillian	Adam Pintar/Will Guthrie	Hood College	Simulation study of an automated threshold selection for Poisson process extreme value models
ITL/CLT	Lamp	Curtis	Mark Przybocki/Mary Theofanos	Shippensburg University	Quantifying Latent Fingerprint Preprocessing
ITL/CLT	Landen	Matthew			Chaining the Cloud, The C-Force's Cryptographic Hash-Chaining Logging Approach
ITL/CLT	Massey	Joshua	Lofti Benmohamed/Frederic de Vaulx	University Maryland Baltimore County	C-Force Enterprise: Towards an Implementation of NCCP Cloud Metrics Model
ITL/CLT	Mayer	Justin	Judy Terrill	University District Columbia	Investigating the mechanics of failure through visualization
ITL/CLT	McGovern	Emily	Lily Chen/Meltem Sonmez Turan	University Maryland Baltimore County	Analyzing the permutation testing methods of NIST SP 800-90B
ITL/CLT	Murphy	Joie	Spencer Breiner	College of NJ	Implementing distributed interfaces: tools from natural language and mathematics
ITL/CLT	Pan	Jane	Hari Iyer/Steve Lund	University Maryland Baltimore County	Impact of Model Uncertainty on Statistical Inferences
ITL/CLT	Patel	Ankur	John Lu	University Maryland College Park	Evaluation of a Plenoptic Camera for Capturing 3D Footwear Impressions
ITL/CLT	Ratliff	Zachary	Rick Kuhn/Raghu Kacker	Texas Engineering Experiment Station	Measuring the Combinatorial Coverage of Software in Real Time
ITL/CLT	Reed III	Carroll	Scott Rose	Bowie State University	Scan and Analysis of HTTPS Certificates Used in the .gov Domain
ITL/CLT	Rodriguez, Jr.	Jose	Kerry McKay	Texas A&M International University	Health Tests of Entropy Sources on Arduino
ITL/CLT	Rogers	James	Paul Black	University Maryland Baltimore County	Injection Preservation: Testing Code with Injected Vulnerabilities for Expected Results
ITL/CLT	Smith	Ryan	Derek Juba/Walid Keyrouz	SUNY Binghamton	Accelerating -D Trees for Nearest Neighbor Search in Walk-on-Spheres
ITL/CLT	Smith	Steven	Thao Nguyen	University Maryland Baltimore County	Calculation of Exclusion Zones for Radar Protection in the 3.5 GHz Spectrum Band
ITL/CLT	Sriram	Vinay	Judy Terrill	Stanford University	Sampling Techniques to achieve Color Fidelity and Anti-aliasing in the Conversion of Cubic Maps to Spherical Maps for Virtual Environments
ITL/CLT	Strange	Sean	Anirudha Sahoo	Millersville University of Pennsylvania	Developing and Testing the Spectrum Access System: Path to Effective Spectrum Sharing
ITL/CLT	Sutton	Kyle	Peter Bajcsy	Howard Community College	Inside a Meteorite: Volume Estimation from the Segmentation of Cross-Sectional Images

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ITL/CLT	Tilva	Rohan	Lotfi Benmohamed/Frederic de Vaulx	Johns Hopkins University	C-Force Enterprise: A Model-based Definition and Management of Cloud Metrics
ITL/CLT	Vargas	Daniel	Martin Herman	St. Mary's University of Texas	Forensic Analysis Automation: Determining Footwear Image Quality Using Machine Learning
ITL/CLT	Wilkes	Matthew	Yang Guo	George Mason University	Developing a Mininet Test Suite for Software Defined Internet Exchange (SDX) Research
ITL/CLT	Xiong	Xinyu	Vincent Hu	City College on NY	Access Control Rule Logic Circuit Simulation (ACRLCS)
MML - MatSci/NCNR	Schankler	Aaron	Paul Kienzle	Haverford College	Refining a Markov Chain Monte Carlo Algorithm for Fitting Neutron Reflectometry Data
MML - MatSci/NCNR	Nguyen	Ai	Christopher M Stafford	Montgomery College	A performance of water and light: Characterizing water purification membranes using ellipsometry
MML - MatSci/NCNR	Elquist	Aline	Jonathan Guyer	Boise State University	New Models for Electrochemical Systems
MML - MatSci/NCNR	Correa-Hernandez	Andres	Eric Cockayne	Boise State University	Density Functional Theory Studies of Nanoporous Materials
MML - MatSci/NCNR	Gayle	Andrew	Robert Cook	Duke University	Nano-Scale Strain Mapping in Three Dimensions
MML - MatSci/NCNR	Moskalenko	Andrey	F. Yannick P. Congo	Purdue University	Developing the Cloud of Reproducible Records (CoRR) and evaluating its performance compared to existing tools
MML - MatSci/NCNR	Ayala	Anthony	Jacob Tarver	University Maryland College Park	Selective gas adsorption in metal organic frameworks
MML - MatSci/NCNR	Dasgupta	Anushka	Jonathan Guyer	Princeton University	Evaluating the Accuracy of Phase Field Codes Using Community-Developed Standard Benchmark Problems
MML - MatSci/NCNR	Panigrahi	Atman	Edwin Chan	University Pennsylvania	Investigation of Salt Transport of Model Polymer Thin Films Via Electrical Impedance Spectroscopy
MML - MatSci/NCNR	Schuberth	Austin	Dilip K. Banerjee	Kansas State University	Finite Element Modeling
MML - MatSci/NCNR	Plavchak	Christine	Ryan Nieuwendaal	Washington & Jefferson College	Determination of 1H NMR spin diffusion coefficients via standard P3HT-PCBM bilayer films
MML - MatSci/NCNR	Hugh	Daevin	Thomas Gnaupel-Herold	University Maryland College Park	Characterizing and Verifying Parameters for Two New Mechanical Systems Through the Multiaxial Deformation of Automotive Sheet Metal
MML - MatSci/NCNR	Villa	Danielle	Qing Huang	Eastern Washington University	Neutron Scattering studies of the Crystal and Magnetic Structures of Molecular Magnets
MML - MatSci/NCNR	Anderegg	David	Daniel Siderius 1	Virginia Polytechnic Institute and State University	Developing a System to Encode Multicomponent Adsorption Isotherms for Standard Reference Data Use
MML - MatSci/NCNR	Scott	Douglas	Katie Weigandt	University Delaware	Structural and Mechanical Characterization of HPMC/SDS Aggregation through Rheological and Neutron Scattering Measurements
MML - MatSci/NCNR	Nusinovich	Edward	Shengyen Li	University Maryland College Park	The application of data mining techniques for efficient material design
MML - MatSci/NCNR	Lee	Erica	Aaron Forster	University Maryland College Park	Durability of Carbon Nanotube Reinforced Alumina Fiber - Epoxy Composites
MML - MatSci/NCNR	McCann	Gordon	Harold Hatch	Gettysburg College	Simulation of Superquadric and Supertoroid Particles to Examine the Effects of Particle Shape upon Self-Assembly Behavior
MML - MatSci/NCNR	Boigenzahn	Hayley	Debra Audus	Worcester Polytechnic Institute	Using Molecular Dynamics to Investigate the Structure of Polyelectrolyte Micelles
MML - MatSci/NCNR	Jeon	Heetae	Jirun Sun	University Maryland College Park	The Unique Functions of Urethane dimethacrylate in Photo-copolymerization with an Ether-based Divinylbenzyl Monomer
MML - MatSci/NCNR	Hunt-Isaak	Ian	Steven Howell	Oberlin College	Small Angle Scattering Calculator for Periodic Boundary Conditions.

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MML - MatSci/NCNR	Boligitz	James	Eric Lass	Temple University	Investigation of phase equilibria in binary Co-W surrounding the μ-phase via mechanical alloying
MML - MatSci/NCNR	Gayvert	James	Alexandros Chremos	Le Moyne College	Molecular Dynamics Study of the Conformational Properties of Polymers in an Explicit Solvent and the Identification of the θ-Temperature
MML - MatSci/NCNR	Collini	John	Brian Bush	Rochester Institute of Tech	Nanomechanical time-dependent properties of PEG Hydrogels
MML - MatSci/NCNR	Huff	Jonathan	Douglas T. Smith	Boise State University	Software Development for a Precision Nanoindenter
MML - MatSci/NCNR	Lagnese	Joseph	Marcus Mendenhall	University Maryland Baltimore County	Analyzing the Analyzer: A Monte Carlo Investigation of X-Ray Diffraction Fits Generated by TOPAS5
MML - MatSci/NCNR	Stracka	Kailey	Daniel Siderius 2	University Maryland College Park	Developing a System to Encode Multicomponent Adsorption Isotherms for Standard Reference Data Use
MML - MatSci/NCNR	Stetsyuk	Karina	Lucas Hale	Hood College	Adding automated uncertainty estimates to temperature- and pressure-dependent property calculations of iron from molecular dynamics
MML - MatSci/NCNR	Mullin	Kathleen	Kimberly A. Tryka	Illinois Institute of Technology	Enabling Discovery of Materials Science Resources Through Robust Metadata Records
MML - MatSci/NCNR	Singer	Lauren	Nicholas Schaub	Bucknell University	Engineering a Low Cost, Open Source Electrospinning System for Nanofiber Production
MML - MatSci/NCNR	Gonzalez-Lopez	Lorelis	Christopher Liman	University of Puerto Rico	Using capillary force lithography to make oriented polymer nanogratings
MML - MatSci/NCNR	Pasco	Madeleine	Erkan Senses	Rose-Hulman Institute of Tech	The effect of nanoparticle architecture and softness on the mechanical properties of the composite polymer
MML - MatSci/NCNR	Bleakney	Matthew	Huong Giang Nguyen	University Maryland Baltimore County	Determining and comparing skeletal density of NIST RM-8852 from different gas measuring techniques/principles
MML - MatSci/NCNR	Wade	Matthew	Thomas Rosch	Case Western Reserve University	Calculation of Radial Distribution Functions using Histogram and Spectral Monte Carlo Methods on a Graphical Processing Unit
MML - MatSci/NCNR	Locke	Michael	Steven Mates	University New Hampshire	Characterizing Material Behavior Via High-Rate Mechanical Testing Using a Split Hopkinson Pressure (Kolsky) Bar and Pulse Heating System
MML - MatSci/NCNR	Super	Nathan	William Ratcliff	College Wm Mary	BLAND UI: User Friendly Neutron Diffraction Analysis
MML - MatSci/NCNR	Luu	Norman	Lucas Hale	Northwestern University	Property Calculations Within the Interatomic Potentials Repository Framework
MML - MatSci/NCNR	Neves	Paul	Nicholas Butch	University Maryland College Park	Designing an AC Magnetic Susceptometer Measurement Technique in Conjunction with High Pressures and Low Temperatures in Neutron Beam Experiments
MML - MatSci/NCNR	Borah	Preetom	Thomas Forbes	Wooster College	Optimization of thermal desorption direct analysis in real time mass spectrometry (TD-DART-MS) for the detection of illicit narcotics
MML - MatSci/NCNR	Wu	Richard	Daniel Sunday	University TX Dallas	Enhanced Safety Analysis Code Suits for the Reactor Design at NCNR
MML - MatSci/NCNR	Leos	Richard	Zeyun Wu	Texas A&M University Kingsville	Morphology and Miscibility: Characterizing A-B-A/B'-C Triblock-Diblock Copolymer Blends
MML - MatSci/NCNR	Bonk	Ryan	RobertWilliams	Le Moyne College	Optimization Study on the Cold Neutron Source for a Proposed LEU Reactor at NIST
MML - MatSci/NCNR	Fangmeyer	Ryan	Mike Middleton	North Carolina State University	System Control: Upgraded Refrigerator
MML - MatSci/NCNR	Isaac	Samantha	Leland Harriger	West Virginia University	Monte-Carlo Exploration of Focused Neutron Guide and Monochromator Geometries
MML - MatSci/NCNR	Underwood	Samuel	Justin Gorham	Reed College	Silver Nanoparticle-embedded Textiles: Preparing and Characterizing a Model System

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MML - MatSci/NCNR	Hood	Sarah	Benjamin Burton	Hood College	Domain Structures and Dynamics of Polar Ordering in Pb(〖Sc〗_(1/2) 〖Nb〗_(1/2))O3 with Pb-O Divacancies
MML - MatSci/NCNR	Smith	Sarah	Shin Muramoto	University of Kentucky Research Foundation	Potential Age Dating of Fingerprints using Time-of-Flight Secondary Ion Mass Spectrometry: Looking at the Diffusion of Fatty Acids on Model Surfaces that Mimic Real World Surfaces
MML - MatSci/NCNR	Brooks	Sydney	Amanda Forster	West Virginia University	Fiber Trace Evidence: Quantification of Sample Bleaching During UV-vis Microspectrophotometry
MML - MatSci/NCNR	Barret	Timothy	Mark Iadicola	University New Hampshire	Uncertainty of the Impulse Excitation Technique
MML-ChemBio	Bezio	Aaron	Jeffrey Hudgens	Gettysburg College	Development of the Next Generation of Hydrogen/Deuterium Exchange Mass Spectrometry Apparatus
MML-ChemBio	Lee	Abigail	Jeanice B. Thomas	University Maryland College Park	Determination of Vitamin C in NIST Food-Matrix Standard Reference Materials
MML-ChemBio	Tran	Anh	Lee Yu	University Maryland Baltimore County	How Safe is Our Ginger? A Study of Arsenic Species in Standard Reference Material (SRM 3398) Ginger Rhizome
MML-ChemBio	Martin	Ann Marie	Tom Allison 2	Mount St Mary's University	Optimization of 3D Molecular Structures for the NIST Chemistry WebBook
MML-ChemBio	Collet	Cayla	Richard Cavicchi	West Virginia Wesleyan College	Protein Aggregation: Characterizing Particles Formed in Therapeutic Protein Drugs
MML-ChemBio	Galvin	Connor	Travis Gallagher	Miami Dade College	Exploring a Novel pH-based Strategy for Protein Crystallization
MML-ChemBio	Hernandez	Cristopher	Lisa Kilpatrick	University Maryland College Park	Observing Trypsin-Catalyzed Transpeptidation Products Using UHPLC-MS
MML-ChemBio	Routkevitch	Denis	Jeffrey Kim	Johns Hopkins University	Analysis of metals in electronic cigarette vapor
MML-ChemBio	Cross	Ebony	Kenneth D. Cole	Capitol Technology University	Bioinformatic Analysis for the Standardization of Mouse Cell Line Authentication
MML-ChemBio	Jin	Emily	Mark Lowenthal	Columbia University	Engineering Biology, Using Bioinformatics to Predict N-Linked Glycosylation Sites in Proteins
MML-ChemBio	Knobloch	Emmie	Diane Bienek	Smith College	Assessing Standard Assays for Cytotoxicity of Dental Materials
MML-ChemBio	Rich	Graham	Nathan Mahynski	Virginia Polytech Inst State University	Understanding the impact surface roughness has on gas adsorption
MML-ChemBio	Bier	Imanuel	Edward Sisco	Augsburg College	Understanding the Effects of Spices in Homemade Explosives Detection by Ion Mobility Spectrometry (IMS)
MML-ChemBio	Young	Jessica	Vitalii Silin	University Maryland College Park	Study of Interaction of Peptides with Tethered Bilayer Phospholipid Membranes
MML-ChemBio	Shevchuk	Mariya	Tom Allison	University Maryland College Park	Optimization of 3-Dimensional Chemical Structures for NIST Chemistry WebBook
MML-ChemBio	Morse	Matthew	T N Bhat	Universityersity of North Florida	Automatically Generated Terminology and Scalable Webtools for Semantic Searching
MML-ChemBio	McDonald	Natalie	Wyatt Vreeland	University Maryland Baltimore County	Characterization of protein aggregation using Asymmetric Flow Field Flow Fractionation (AF4) and Multi-Angle Light Scattering (MALS)
MML-ChemBio	Patel	Nimit	Tom Allison 1	University Maryland College Park	Optimization of 3-Dimensional Molecular Structures for NIST Chemistry WebBook
MML-ChemBio	Knowlden	Steven	Joseph T. Hodges	University Maryland College Park	A Comparative Analysis of Mercury Generator Certifications, Past and Present
PML-EE	Guo	Anthony	Oleg Kirillov	State University of New York Binghamton	Metrology for Organic Spintronic Devices
PML-EE	Vasilyev	Anton	Jason Underwood	University of Delaware	Evaluating Distortion Correction Methods for High-Resolution Digitizers
PML-EE	Chiu	Arlene	Dean Jarrett	University of Maryland College Park	Temperature Coefficients on Guarded Hamon Transfer Standards
PML-EE	Gamble	Claudia	Richard Steiner	University of Maryland College Park	Testing Smart Watthour Meter Accuracy
PML-EE	Wade	Collin	Emily Bittle	Washington University in St. Louis	The electronic stability of polymer dielectrics for use in low temperature measurements of organic electronics
PML-EE	Rhodes	Corey	Joseph Kopanski	West Virginia Wesleyan College	Designing a Charge-Based Capacitance Measurement Circuit for Interfacing with an Atomic Force Microscope
PML-EE	Liu	Eileen	Ravikiran Attota	University of Maryland College Park	Using MATLAB in the Development and Optimization of Nanoscale Measurement Techniques
PML-EE	Gurara	Firehiwot	Charles Cheung	Montgomery College	Magnetic Field Uniformity Through Pole Face Optimization
PML-EE	Montgomery	Karl	Yaw Obeng	University of Maryland College Park	Broadband Spectroscopic Characterization of Low-k Dielectric Thin Films for Micro- and Nanoelectronic Applications
PML-EE	Motabar	Lily	Darwin Reyes	University of Maryland College Park	3D Printing Microfluidic Devices with Electronic Functionalities
PML-EE	Goebel	Michael	Tom Lebrun	State University of New York at Binghamton	Locking Lasers Using a Digital Servo
PML-EE	Verrill	Nathan	Allen Goldstein	Andrews University	Power System Synchrophasor Data Impairment using Labview
PML-EE	Phan	Nhi	Joe Rice	Worcester Polytechnic Institute	The Hadamard Transform Hyperspectral Image Projector
PML-EE	Davis	Robert	John Lawall	University of Maryland College Park	Automation of an Optical Pressure Standard: Dante's Divine Comedy of Pressure
PML-EE	Buttles	Robert	Jacob Ricker	University of Colorado Boulder	Broadly Tunable, Narrow Linewidth Lasers

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PML-EE	Chavali	Sai Meghasena	Jeffery Nico	University of Maryland College Park	Measuring the wavelength of a cold neutron beam for a neutron lifetime experiment
PML-EE	Nikolaitchik	Theodore	Suijitra Pookpanratana	University of Maryland College Park	Molecular Interfaces and its Impact on Electronic Functionality
PML-EE	Zirkle	Theodore	Meghan Shilling	Walla Walla University	Experiment Design to Analyze the Effect of Roughness and Machining Operations on Light-Based Three-Dimensional Coordinate Measuring Devices
PML-PL	Barner	Lindsey	Andras Vladar	Messiah College	Machining of Fluidic Structures with Helium Ions
PML-PL	Brandt	Samuel	Michael Huber	Valparaiso University	Measurement of Schwinger Scattering in Silicon
PML-PL	Brown	Samuel	Maritoni Litorja	Carleton College	Standardizing Firefly Luminescence
PML-PL	Edgerton	Joshua	Denis Bergeron	Appalachian State University	Quantification of PET Imaging Using NIST-calibrated Radionuclide Sources
PML-PL	Graybill	Joshua	Charles Clark	University of Maryland College Park	Excimer-based Neutron Detection using Far Ultraviolet Noble Gas Emission
PML-PL	Hanson	Joshua	Joseph Tan	Clemson University	Capturing Highly Charged Ions in a Radio-Frequency Paul Trap
PML-PL	Hastings	Hannah	Cameron Miller	Bryn Mawr College	Not All AC Power Supplies Are Equal, According to an LED Source
PML-PL	Lindsay	Maxwell	Angela Hight-Walker	University of Pittsburgh	Controlled carbon nanotube functionalization for assessing origin of Raman D-band components
PML-PL	McClung	Samuel	Keith Gillis	Stevens Institute of Technology	Unusual Phenomena in Convective and Sonic Gas Flows
PML-PL	Paseltiner	Daniel	Ian Spielman	Bates College	Development of a Digital Holographic Microscope for Imaging Bose-Einstein Condensates
PML-PL	Riley	Benjamin	Heather Chen-Meyer	Universityersity of Kentucky	An Evaluation of a Dual-Energy Method for CT Imaging
PML-PL	Schafer	Benjamin	Scott Dewey	Hamilton College	Neutron Polarization Measurement on the NG-C Beamline for aCORN
PML-PL	Townley-Smith	Keeley	Gillian Nave	Lamar University	Line identification and level analysis of Ti II in the ultraviolet region
PML-PL	Valdillez	Robert	Pieter Mumm	North Carolina State University	Measuring the Neutron Spectrum of 250Cf with a Time of Flight Measurement
PML-PL	Walecki	Peter	Ronald Tosh	Florida Atlantic University	Radiation Dose Metrology through Water Calorimetry
SCO	Gilpin	Anna	Clare Allocca, Sumona Sarkar	West Virginia University	What is the Meaning of Life?: Terminology and Measurement Assurance of Biotechnology Standards
Special Programs	Resnick	Benajmin	Paul Zielinski	Case Western Reserve University	Marketing and Licensing of Microscopy Technology
Special Programs	Emelike	Joseph	Reva Schwartz	Bowie State University	Golden Cross Section
TPO	Ekwuru	Miriam	Paul Zielinski	Coppin State University	Commercialization of Inventions in the fields of Bio-manufacturing and Medical Devices