UF | UNIVERSITY of FLORIDA

***Anderson Laboratory – Chemical Engineering***

Current research efforts focus on the study of advanced electronic materials processing issues, particularly those related to thin film deposition systems. The Anderson laboratories include 6 major CVD systems and an MBE deposition system. In particular, a custom-designed DVD system is dedicated to the growth of barrier materials using organometallic precursors. The system includes an rf-heated reactor capable of operating at low pressure, and an aerosol delivery system for transporting non-volatile precursors. This system has been used in precursor screening as well as film growth for barrier efficacy studies.

The lab is also equipped with a 2-chanber ALD-CVD system. The first chamber is a low-volume ALD reactor that can operate at low pressure to 700° C with automatic flow switching. Films deposited in this chamber can be transferred via a load-lock to a second chamber designed for CVD or ALD Cu deposition, thus preventing exposure to the ambient.

A third chamber if interest is a vertical upflow, impinging jet CVD reactor that is interfaced to an spectrometer to perform in situ Raman scattering and laser-induced fluorescence studies. The reactor is mounted on an x-y-z translation stage thus allowing composition and temperature profiles to be measured. This is believed to be a unique system.

A new 3-chamber UHV characterization system is now under construction to better understand how molecules absorb and decompose on substrates. It incorporates a preparation chamber to dose a substrate with a precursor, which can then be transferred to a second chamber to probe the adsorbed state of molecules using ATR. The third chamber is equipped with LEED optics and AES system as well as TPD. This system will be useful in understanding adsorption and reaction mechanisms.

The Anderson lab also has a number of film characterization tools, such as FTIR, micro Raman and SEM.

***Asthagiri Laboratory – Chemical Engineering Department***

Aravind Asthagiri's research involves the simulation of novel materials from an atomistic level. He uses a multiscale modeling approach to link atomic-level information to observable macroscopic properties. The accurate simulation of material properties is critical for insight on the underlying phenomena and design of novel materials.

Professor Asthagiri has his own 64 dual processor nodes (CEC cluster) and access to the University of Florida High Performance Computing Center (www.hpc.ufl.edu ), which has over 1600 cpus and a projected 6 Tflops with an planned expansion to over 2400 cpus and 9 Tflops.

***Center for Manufacturing Innovation*** *(CMI)*

Manufacturing at UF focuses on performing state-of-the-art research to produce innovative manufacturing and surface technologies. These technologies enable improved product performance and breakthroughs in water, food production, energy, aerospace, and healthcare systems. Students from the high school to graduate levels are trained to have strong analytical/computational modeling capabilities coupled with sound experimental techniques and data analysis skills.

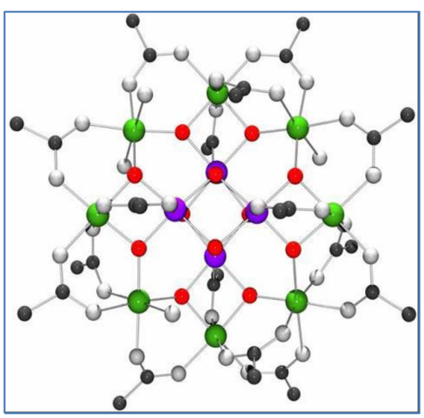
While the historical focus has been macro-scale manufacturing applications, with the addition of new faculty and facilities, new activities at the micro- and nano-scale are underway. Current research areas include:

- 3D printing with applications to human tissue fabrication
- magnetic field-assisted finishing
- micro- and nano-manufacturing
- high-performance machining of advanced materials
- modeling and sensing of machining processes

As you browse our site, we look forward to receiving your feedback, answering your questions, and learning how we can work together to improve global manufacturing capabilities.

***Christou Group – Chemistry Department***

The Christou group is a synthetic and physical inorganic group with strong interests in synthesis and characterization of multinuclear transition metal complexes. We characterize our samples using IR, paramagnetic NMR, electrochemistry, magnetism studies, mass spectroscopy and X-ray crystallography.



The Christou group at the University of Florida Chemistry Department has all the necessary resources for the synthesis and characterization of transition metal compounds, and their study by a wide range of techniques. The group office and laboratory space was renovated for the move of the P.I. to the University of Florida from Indiana University, Bloomington, in the summer of 2001.

***Laboratory***

The group's personnel are housed in four laboratories fully equipped for synthetic chemistry and capable of accommodating a total of 16-18 people. Each laboratory is fitted with efficient fume hoods (one per person) and spacious bench space for safe and efficient synthetic chemistry. Most fume-hoods are equipped with inert-atmosphere Schlenk lines to allow synthetic chemistry under oxygen- or moisture-free conditions, as required. The student desks are physically separated for safety from the laboratory space; they are in a separate area but the connecting wall has windows so that they can look into the laboratory. All glass-fronted storage cabinets in the laboratories are ventilated. Storage of solvent bottles is in metal cabinets.

***Computer***

The Christou group possesses several modern PC computers dedicated to research use, including manuscript preparation, graphics, fitting of magnetic data by various commercial (Sigmaplot) and locally-written (MAGNET) software packages, and ZILSH theoretical calculations. These computers also are part of site-licenses providing access to the Cambridge Structural Database (CSD) and the Chemical Abstract Service (CAS Online) for efficient searches of the crystallographic and chemistry literature, respectively. Computers also control the FT-IR and UV/vis spectrophotometers, the electrochemical apparatus, and the SQUID magnetometer. DFT calculations are carried out on high-capacity mainframes at the University of Florida's High-Performance Computing (HPC) Center (see http://hpc.ufl.edu), where Christou Group students have individual accounts for running more arduous calculations.

***Office***

The P.I. and his secretary share an office cluster down the hallway from his laboratories. Postdoctoral Associates have desk space in a small office adjoining one of the laboratories. A conference room is at one end of the inorganic chemistry floor, and is available for group meetings and small lectures by any inorganic group.

***Environment***

The Chemistry Department of the University of Florida is a large (~45 faculty) department with an international research reputation spanning all of its seven divisions (Organic Chemistry, Inorganic Chemistry, Biochemistry, Analytical Chemistry, Physical Chemistry, Quantum Theory Project, Polymer Chemistry). This is result of the stature of its research faculty and the quality of its graduate students and postdocs. It has a large PhD program, the third largest producer of chemistry PhD graduates in the USA (C&E News, November 23, 2009). It recruits excellent students from around the world, which has allowed the P.I., for example, to have accelerated his research substantially since moving there in the summer of 2001. The quality of the PhD students and postdoctoral fellows he was able to attract to his group are the main reason for the highly satisfactory research output of the Christou group in recent years, which, for example, published 138 peer-reviewed papers in the five-year 2005-2009 period.

(http://www.chem.ufl.edu/~christou/group/)

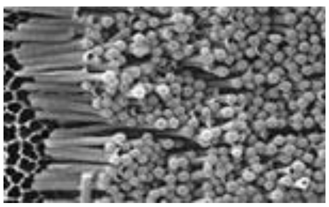
The Chemistry Department maintains many of the equipment and resources required by the P.I.'s group to carry out the proposed research, complemented with the equipment within the Christou group itself (see Equipment page). The P.I. also has a strong rapport with his chemistry colleagues, and thus has access to internationally respected experts in areas of relevance to the proposed research.

***Hagelin-Weaver Laboratory***

We take a multidisciplinary approach to heterogeneous catalysis, using principles from organometallic chemistry, quantum chemistry, surface science, and reactor design and reaction kinetics. The objective of our research is to obtain a fundamental understanding of heterogeneous catalysis at the atomic level, focusing on reactions that are environmentally advantageous.

Dr. Hagelin-Weaver has adequate office space with an office computer and approximately 1000 square feet of laboratory space. At least 25% of the laboratory space will be available to the proposed research.

***Martin Research Group***



Research interests in the Martin group are in the areas of Materials and Analytical Chemistry with special emphasis on nanomaterials and the bio/nano interface. Our research group has pioneered a versatile approach for preparing nanomaterials called the template method. We have been exploring applications of template-prepared nanotubes and nanotube membranes in biosensors and separations. We are also interested in electrochemistry at nanoscopic electrodes and in electrochemical energy storage and production.

***McElwee-White Research Group – Chemistry Department***

Our research involves applications of organometallic chemistry to problems in materials deposition, methodology for organic synthesis, and catalysis. Recent areas of research include organometallic precursors for the chemical vapor deposition (CVD) of inorganic films that are of interest for manufacture of semiconductor devices, heterobimetallic catalysts for the electrochemical oxidation of alcohols with applications to direct methanol fuel cells, and catalytic carbonylation of amines as an alternative to the use of phosgene and its derivatives.

The McElwee-White group has laboratory and bench space for 15 people, Schlenk lines, and standard small pieces of equipment (ovens, refrigerators, circulating chillers, analytical balances, etc.) along with major items described in Appendix 12.

**Merz Laboratory - Quantum Theory Project**

***Laboratory***

The KMM Lab has ~1200 sq. ft. of laboratory space.

***Computers***

We have excellent computational facilities available to us to do the proposed research. Each student/postdoctoral fellow has access to a desktop machine and/or a laptop (either a Mac or Linux box). The Merz group has a 76 node AMD Opteron (dual processors; 4Gb RAM)) cluster and a newer generation 16 node Opteron cluster (8 cpus per node; 16 Gb RAM) with Tbs of disk space in a RAID system shared with the university HPC center. We are in the process of installing a 16 node Opteron cluster (12 cpus per node; 32Gb per node). All resources will be available to this project to do numerically intensive calculations. Indeed, AF-QM/MM run using Gaussian 09 makes excellent use of our shared memoory parallelism (2-12 cpus per node) greatly speeding up these calculations. Moreover, the parallelism achieved by running one fragment per node is quite significant as well allowing us to tackle systems with thousands of atoms in a reasonable amount of time. We have access to several multi node (details can be found here: http://wiki.hpc.ufl.edu/index.php/Operating_Environment) Linux clusters, which we share with the university at the UF-HPC center. If necessary, we will apply for supercomputer time to ensure that we have access to state-of-the-art computing facilities to carry out NSF supported research. However, we have found that with our local resources that supercomputer center resources are less critical to our work. In short the computer resources available to us are more than sufficient to carry out all of the proposed research.

***Software***

All NMR calculations will be carried out using DivCon (a linear-scaling semiempirical code) or with Gaussian 03/09.

***Office***

The PI has a ~200 sq. ft. office.

***Other***

We have an excellent theoretical group here at UF contained within the Quantum Theory Project. Discussions with QTP members will clearly benefit the present proposal. UF also is one of the schools (Florida State is the lead institution) involved in the High Field Magnet Lab sponsored by the NSF. This creates a critical mass at UF for NMR based research and clearly this proposal will benefit from these interactions. In short, UF has an excellent environment for theoretical and NMR oriented research on biomacromolecules.

***Multi-functional Integrated System Technology (MIST) Center***

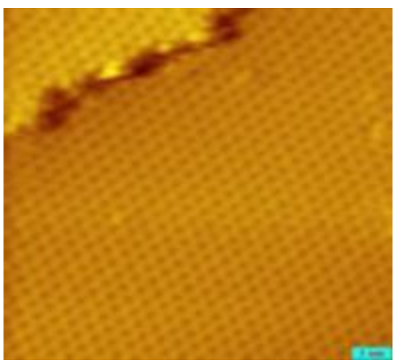
The University of Florida's Multi-functional Integrated System Technology (MIST) Center will play a leading role in researching the next generation of "smart" electronics funded by a National

Science Foundation program that combines federal money with industry investments in strategic research.

As a designated Industry/University Cooperative Research Center, the MIST Center will receive over $880,000 from the NSF and upwards of $4 million from industry and government partners to help power the "Internet of Things."

In the last 30 years, the Internet revolution has completely changed how we communicate, exchange money and explore the world. Access to the Internet has evolved from the desktop computer to hand-held - and now wearable - devices. Soon, engineers envision an interconnected cyber-physical world, dubbed an "Internet of Things." The MIST Center will research the materials, sensors, actuators, power sources and electronics that are expected to drive this new era.

## ***Weaver Lab – Chemical Engineering***



Our research focuses on advancing the molecular-level understanding of chemical reactions occurring on solid surfaces. Such reactions are fundamental to heterogeneous catalysis and semiconductor processing, yet remain poorly understood at the molecular level. We investigate surface chemical reactions experimentally using sensitive surface spectroscopic techniques combined with reactive beam scattering in ultrahigh vacuum (UHV). This is a powerful approach for probing the mechanistic details of surface reactions as it enables one to prepare atomically clean surfaces and to induce chemical reactions on these surfaces in a highly controlled manner. The combined use of reactive beam scattering and surface analysis also provides comprehensive information about surface chemical reactions since both the gaseous and surface reaction products are analyzed with high resolution. We also use in situ scanning tunneling microscopy (STM) to obtain real-space images of atoms on solid surfaces. Investigations with STM enable us to examine how different, local arrangements of atoms influence the reactivity of a solid surface, and, conversely, how chemical reactions modify surface structures over nanometer dimensions.

### ***Laboratory:***

Co-PI Weaver has 1200 sq. ft. of laboratory space with cooling water and sufficient electrical power.

### ***Computers***

Eight Pentium minicomputers, and one server with dual xeon processor and RAID array.

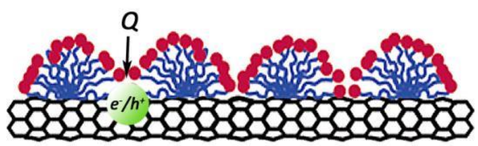
### ***Office:***

Weaver's office is located in close proximity to the laboratory.

***Other Resources:***

The College of Engineering has a fully equipped machine shop and the Department of Chemical Engineering employs a fulltime maintenance specialist for laboratory repairs and modifications.

***Ziegler Laboratory***




As technology rapidly shrinks toward the nanometer length-scale, understanding how dimensionality affects materials properties has become increasingly important. At the nanoscale, electron interactions are restricted resulting in unique properties that differ from the macroscopic world. Our goal is to synthesize nanomaterials exhibiting unique properties, understand and manipulate their properties, and integrate them into critical new devices and inventions that will affect microelectronics, manufacturing, healthcare, biotechnology, energy, and materials science.

***University of Florida Major Analytical Instrumentation Center (MAIC)***

Materials and structural characterization of nanomaterials for this project will be performed at the Major Analytical Instrumentation Center (MAIC) located on the University of Florida campus. MAIC is a materials characterization and analysis facility established to provide analytical support for Florida's scientific and engineering community in meeting the challenge of technology development. MAIC is a user oriented facility that provides service to the University of Florida, the state university system (SUS), and the industrial and commercial community. The facilities at MAIC relevant to this project include:

- Focused Ion-Beam (FIB): FEI Dual-Beam Strata DB235
- Transmission Electron Microscopes (TEM): JEOL 2010F (Field Emission Scanning Transmission Electron Microscope/ TEM STEM-Z, EDS, EELS, Remote Operation Capabilities) and a JEOL 200CX (Analytical Electron Microscope/ TEM, STEM)
- Scanning Electron Microscopes (SEM): FEI XL-40 FEG-SEM (Field emission gun Scanning Electron Microscope with Oxford EDS system), JEOL SEM-6400, and a JEOL 6335F (Field Emission Scanning Electron Microscope/ SEI, BEI, EDS, Remote Operation Capabilities)
- Atomic Force Microscopes (AFM): Digital Instruments Multimode Nanoscope III and a Digital Instruments Dimension 3100
  X-Ray Photoelectron Spectrometer (XPS): Perkin Elmer 5100 XPS System (XPS/ESCA, ARXPS)
- X-Ray Diffractometer (XRD): Philips APD 3720
- Fourier Transform Infrared Analyzer (FTIR): Nicolet 20 SX

## [University of Florida Nanofabrication Facility (UFNF)]

The University of Florida has recently invested $6 million in establishing a nanofabrication facility. A variety of tools including an electron beam lithography tool, reactive ion etching, contact photolithography, and sputter deposition have been acquired and housed in two separate clean room facilities in the Electrical and Computer Engineering (ECE) and Physics departments. The facilities at UFNF relevant to this project include:

- Lithography: Raith 150 E-beam Lithography, Karl Suss MA6 contact aligner, Karl Suss MJ55 contact aligner, Karl Suss MA4 contact aligner, 3 Headway spin coaters (can coat up to 4 inch wafers), Other related lithography equipment
- Furnaces and Chemical Vapor Deposition: BTI atmospheric tube furnace system, BTI LPCVD systems, Heatpulse 2100 rapid thermal annealer (RTA), STS 310PC PECVD for oxide and nitride deposition
- Metal Deposition: KJL CMS-318 Multi-target Sputter Deposition, Tellmark E-beam evaporation, Varian 3 pocket E-beam evaporation
- Dry Etching: Plasma Sciences RIE 200W, STS Deep RIE, Tegal 701 RIE, Unaxis Shuttlelock RIE-ICP

UFNF also has all the standard wet processing, wafer preparation, inspection, and characterization facilities.

## *Particle Engineering Research Center (PERC)*

The Research & Development Facility is an integral part of the Particle Engineering Research Center at the University of Florida. It includes state-of-the-art instrumentation for particle characterization and analysis. The 17,000 square foot space includes six analytical laboratories, two processing labs, and a 5000 square foot testbed. The facilities at PERC relevant to this proposal include:

- *Zeta Potential Measurement*: Brookhaven ZetaPlus, Colloidal Dynamics Acoustosizer IIs, Paar Physica Electro Kinetic Analyzer, and Zeta Reader Mark 21• *Chemical Analysis*: Nicolet MAGNA 760 FTIR/FT-Raman microscope, Perkin-Elmer Lambda 800 UV-Vis spectrometer
- *Film Characterization*: NRL C.A. Goniometer with autopipetting and imaging systems, Hysitron Micro Nanoindentor, Woollam EC110 Ellipsometer
- *Raman Spectroscopy*: Reinshaw Invia Bio Raman with excitation from a 785 nm diode laser

***Nanoscience Institute for Medical and Engineering Technologies and the Nanoscale Research Facility***

(NIMET) UF and the Nanoscale Research Facility (NRF) is to provide support for major research center initiatives at the University of Florida (UF) in the areas of nano-and-micro-scale science and technology (NMS&T). Support can be provided in several ways noted below:

- Facility open to all faculty, staff, and collaborators. It provides research space and state-of-the-art equipment for research, education, nanofabrication, and prototype development of nano-materials, MEMS and NEMS devices, and sensors in NMS&T.

NRF's capabilities include:

- Class 100-1000 cleanroom bays for nanofabrication.
- A bio-nano bay in the cleanroom specifically for functionalization of nano-electronic devices with biological molecules, and for nano-toxicology investigations.Electron beam, ion beam, and optical lithography.
- Advanced electron, optical, and surface imaging laboratories.
- Core research laboratories for synthesis, processing, characterization, assembly, testing, and integration of organic and inorganic nanoscale materials, devices and sensors.
- General laboratory space for industry and interdisciplinary research collaborations. • Offices for faculty, staff, students, industrial affiliates, and collaborators.
- Interactive spaces for conferences, informal gatherings, user administration, and surroundings conducive to multidisciplinary interactions.
- Building support and utility handling areas.
- A complete building automation monitoring system to ensure efficient and safe research operations.

NIMET and NRF also provide highly trained technical staff to operate, maintain, and improve facilities, and to educate students in NMS&T techniques and equipment use as part of their education.

***Relevant Advanced Imaging and Nanofabrication Capabilities***

In addition to NRF's conventional commercially-available nanofabrication and advanced imaging capabilities, NRF has developed equipment that provides some unique research advantages. For example, NRF has a new ion beam lithography and processing system that is the only one of its kind in the U.S. that provides:

- FIB Performance. Scanning FIB with spot sizes ~ 8-30nm depending on configuration.
- Ion Beam Lithography**.** Software for sample manipulation over large areas (100 x 100

mm$^2$); stitching and high-speed pattern processing; all with nanometer precision.

- Mass-Separated, Multi-Ion Capability. ExB filter for mass separation of Au, SI, and Ga. Ions. Other Liquid Metal Alloy Ion Sources (LMAIS) sources are available that can provide more than 25 elements in the periodic table.
- Maskless Ion Implantation (II). II of selected ions; 1-40 kV; in situ processing without masking steps; and selected ion species.
- Real-Time Visualization. Scanning ion-induced secondary electron images (high contrast images due to ion channeling) for real-time analysis of sample.
- Surface Functionalization. Damage, implantation, deposition, and ion mixing can produce seedsites with selected ion species for nanowire growth, catalysis, biological functionalization,etc.
- 3-D Localised Patterning and Engineering**.** Programmed lithographic patterning for ion sculpting of micro-fluidic structures, nanopores, etc.. Low energies and ion-cluster sputtering can achieve high-rate patterning with low atomic-mixing and shallow damage effects.
- User Friendly**.** Integrated software controls with an ion beam database for users.

These capabilities are particularly suitable for fabricating complex prototype nano/micro-scale devices because many processing steps can be performed directly without the normal e-beam lithography, exposure, development, evaporation, lift-off, etching, evaporation, etc. that accompany conventional nanofabrication. One of the advanced imaging tools we have is an ultra high resolution SEM with Cathodoluminescence capabilities for getting optical and bandstructure information from samples.

## ***Useful Equipment Items***

### ***LMAIS Sources***

The multi-ion beam lithography and processing system can be used for fabricating some of the complex integrated systems in the nano devices intended to capture all photons. Once the processing simplifications are identified one could identify the desired ion species needed for fabrication and acquire the necessary LMAIS source. (For example, if one had a solar cell or nanoelectronic device that needed Boron doping this could be done with the B LMAIS source, using the nano-scale ion beam directly on the device without any masking or additional lithography steps).

### ***SEM with CLD Capability.***

Cathodoluminescence should be very useful for determining the spectral properties of fabricated nano-structures used for capturing and utilizing solar radiation.

### ***Major Analytical Instrumentation Center (MAIC)***

The Major Analytical Instrumentation Center (MAIC) is a user oriented service facility that provides materials characterization and analysis services, courses and training to the scientific community at the University of Florida. Faculty and graduate students at the various departments in the College of Engineering are the major users of the facilities. Thus, the MAIC adds value to the College of Engineering by contributing to the college and university's mission of research, teaching and service.

The teaching component of the MAIC activities is accomplished through the formal undergraduate and graduate courses offered at MAIC: Analysis of the Structure of Materials (U), Scanning Electron Microscopy and Microanalysis (G), Auger Electron Spectroscopy (G), X-Ray Photoelectron Spectroscopy (G), Transmission Electron Microscopy (G), X-Ray Diffraction (G), X-Ray Analysis of Thin Films (G). The MAIC staff also conducts individual and group training for those instruments and techniques that we don't have a formal course to offer. In addition, a new graduate certificate in materials characterization will be offered through the EDGE program starting in the fall 2008.

The research component of the MAIC activities is covered through the use of the instrumentation at MAIC by the faculty and students users of the facility. Research conducted by the faculty and students in the Colleges of Engineering, Liberal Arts and Sciences, Agricultural and Life Sciences, Dentistry, Design, Construction and Planning, Medicine, Pharmacy, Veterinary Medicine, and the Museum of Natural History, occupies most of the instrument hours at the MAIC. The staff at the MAIC also conducts independent research. Currently Dr. Craciun has two graduate students, and Dr. Bourne has one graduate student, working under their guidance towards their Ph.D. In addition, Dr. Dempere has a Post Doc under her direction working on a research project for the Florida DOT.

The service component of the MAIC activities is represented by the extensive number of hours in instrumentation appointments, education, training and participation in graduate committees provided by the MAIC staff. The increase in the service hours in the past years has been recognized with the 2008 Prudential Financial Davis Productivity Award for doubling the productivity of the center since 2000.