National Lab Day in Mississippi

November 8, 2012

Areas of Potential Collaboration

Materials Panel

Materials Discovery, Design, and Synthesis

- Crystal growth and epitaxy
- Nanoscale synthesis: Carbon-based nanostructures (including graphenes), nanoparticles, catalysts, and tailored films
- Nanofabrication (focused ion beam, electron-beam lithography) of conventional, soft, and hybrid materials
- Next generation materials for batteries, supercapacitors, fuel cells, thermoelectrics, superconductors, photovoltaics, ferroelectrics, catalysis and separations

Materials Under Extremes

- Ultra high temperature/pressure, lightweight structural materials
- Radiation resistant structural materials and nuclear fuels materials
- Strong, impact resistant alloys, ceramics, composites, and concretes.
- Corrosion-resistant materials

Polymers and Composites

- Anionic and free-radical chemical synthesis
- Hierarchical and composite structures
- Opto-electronic functionality in polymers
- Functional and structural carbon fiber and novel precursors

Interfacial Science and Transport

- Solid-fluid interface science and applications to electrical energy storage, corrosion, separations, geoscience and catalysis.
- Electron and photon transport at interfaces
- Designed ligands for targeted isolation, purification and concentration
- Tailored mesoporous carbons, polymers and oxides for selective transport

Advanced Imaging and Characterization

- Ultra-high resolution and in situ electron microscopy
- Advanced scanning probe microscopies and spatially-resolved functional measurements
- Chemical imaging via coupled optical spectroscopy, scanning probes, and mass spectrometry
- Neutron scattering and spectroscopy
- Nuclear magnetic resonance spectroscopy of solids and interfaces
- Mechanical testing and analyses of simple and composite structures under multi-axial loading conditions at high temperatures and stresses.

Materials Theory, Modeling and Simulation

- Multi-scale modeling of materials, including first-principle methods, statistical techniques, and model-Hamiltonian based approaches
- Modeling systems failure and performance

Materials Processing

- Pulse thermal processing, battery processing, and additive manufacturing
- Materials joining and failure analysis

User Facilities at ORNL for Materials Research

- Center for Nanophase Materials Sciences (CNMS) http://cnms.ornl.gov/
- Shared Research Equipment User Facility (ShaRE) http://www.ornl.gov/sci/share/
- Spallation Neutron Source (SNS) and High Flux Isotope Reactor (HFIR) http://neutrons.ornl.gov/
- Oak Ridge Leadership Computing Facility (OCLF) http://www.olcf.ornl.gov/
- Manufacturing Demonstration Facility (MDF) http://www.ornl.gov/sci/manufacturing/mdf.shtml
- Carbon Fiber Technology Facility (CFTF) http://www.cfcomposites.org/cf_technology_facility.shtml

ORNL Materials Centers

- Fluid Interface Reactions, Structures and Transport (FIRST) Center http://www.ornl.gov/sci/first/index.shtml
- Center for Defect Physics (CDP) http://cdp.ornl.gov/
- Consortium for Advanced Simulation of Light Water Reactors (CASL) http://www.casl.gov/

Contacts

Michelle Buchanan, Associate Laboratory Director
Physical Sciences
buchananmv@ornl.gov, 865-574-1144

Phil Britt, Director
Chemical Sciences Division
brittpf@ornl.gov, 865-574-4986

Gene Ice, Director
Materials Science and Technology Division
icege@ornl.gov, 865-574-4065

Sean Smith, Director
Center for Nanophase Materials Sciences
smithsc@ornl.gov, 865-574-5081

Argonne NATIONAL LABORATORY

Theoretical, Computational and Experimental Materials Research

- Theoretical superconductivity, electronic structure and magnetism
- Materials synthesis focus on correlated electron transition metal oxides, chalcogenides, and novel superconductors
- Charge-transfer processes and chemical environment in the vicinity of electrode surfaces
- Chemical, microstructural, and interfacial contributions to ferroic nanostructure behavior
- Synthesis and characterization of molecular materials with novel magnetic, conductive, and catalytic properties; magnetic thin film and superlattice properties
- Computational materials science focus on electronic structure methods and molecular dynamics simulations
- Magnetic vortex system studies in high temperature superconductors
- Theoretical and experimental studies of active self-assembled materials
- Detector development, analytical chemistry, and chemical warfare agent chemistry
- Electrochemical energy storage, lithium battery R&D, battery materials scale-up
- Heterogeneous and homogeneous catalysis & energy conversion

Advanced Characterization and Spectroscopy

- Advanced microstructural characterization
- Scattering investigations on high temperature superconductors, disordered solids and liquids, magnetoresistive oxides, and magnetic surfaces and interfaces
- Synchrotron radiation study of structures and electronic properties of materials
- Scanning probe tunneling and atomic force microcopy; near-field scanning optical microscopy
- Nanoscale fluorescence, diffraction, and transmission imaging

Nanoscience

- Growth and characterization of nanostructured thin films
- Polymeric and bio-templating, nanoparticle synthesis, biosynthesis, molecular beam epitaxy
- Nanofabrication, chemical and biological functionalization of nanoscale materials; electron-beam lithography, focused ion beams, and nanoimprint patterning methods

Nuclear & Environmental Processes

- Heavy element and separations science, interfacial processes, radiochemistry, process simulation & equipment design, pyroprocess development
- Process safeguards, environmental science, nuclear forensics

User Facilities for Materials Research

- Advanced Photon Source
- Center for Nanoscale Materials
- Electron Microscopy Center
- Argonne Tandem Linear Accelerator System
- Argonne Leadership Computing Facility

Contacts

Emilio Bunel
Director Chemical Sciences & Engineering Division
ebunel@anl.gov, 630-252-4383

Michael Norman
Director Materials Science Division
norman@anl.gov, 630-252-3518

Amanda Petford-Long
Director Center for Nanoscale Materials
petford.long@anl.gov, 630-252-5480

Experimental and theoretical programs in fundamental materials research:

Materials discovery, design, and synthesis

- Nanoscale chemical synthesis and assembly, inorganic nanostructures
- Solid state synthesis and growth – superconductors, magnets, thermoelectrics, ferroelectrics, light emitters
- Polymers and hybrid inorganic-polymer composites
- Surface and interfacial chemistry – catalysis, interfacial electronic structure
- Synthesis and processing science – diffusion, nucleation, phase transitions
- Biomimetic/bioinspired functional materials and structures

Advanced Imaging and Spectroscopy

- in situ electron microscopy and x-ray spectroscopy
- Near-field optics and scanning tunneling microscopy
- Time- and spin-resolved photoemission spectroscopy
- Nuclear magnetic resonance of molecules and assemblies, and extension of them to novel applications

Condensed matter physics

- Quantum materials, magnetic materials, spin physics, metamaterials
- sp2-bonded materials and nanostructures, including graphene
- Ultrafast phenomena in materials
- Mechanical behavior of advanced materials, alloys, and nanostructures
- Quantum and statistical mechanical theories of materials

Actinide science

- Solid state physics and chemistry of radionuclides
- Wasteforms

Computation and Theory for Materials Discovery and Understanding

- The Materials Project
- SciDAC Partnership for Excited States in Energy Materials
- Nanoporous Materials Genome

User Facilities at LBNL for materials research

- Advanced Light Source, www-als.lbl.gov
- Molecular Foundry, foundry.lbl.gov
- National Center for Electron Microscopy, ncem.lbl.gov
- Energy Sciences Network, www.es.net
- National Energy Research Scientific Computing Center, www.nersc.gov

LBNL materials centers

- Center for x-ray optics, www.cxro.lbl.gov
- Joint Center for Artificial Photosynthesis, North, solarfuelshub.org
- Glenn T Seaborg Center, actinide.lbl.gov

Contacts

Frances Houle, Director of Strategic Initiatives
Chemical Sciences Division
FAHoule@lbl.gov, 510-495-8135

Jeff Neaton, Acting Director
Materials Science Division
JBNeaton@lbl.gov, 510-486-4527

- Nanomaterials Research including studies that have led to:
  - *MRI contrast agent prototypes,*
  - *functional ferrofluids with medical applications,*
  - *additives in stimuli-responsive, multi-functional adhesives*
  - *nano-dopants for conducting and magnetically responsive polymers, and*
  - *architectural subunits of biologically inspired materials to address areas of military and civilian concern, e.g. chem-bio defense*

- Surface Chemistry including morphology-structure-property correlations in organic electronic material, in particular, photovoltaic polymer materials, at the molecular level.

- Biopolymer and bioinspired polymeric materials include development of self-assembling systems for sensor applications and surface modification for antifouling/antimicrobial performance

- High performance materials, including composites, nanocomposites and nanostructured materials.

- The design of functional polymer surfaces and thin films with applications ranging from antifouling coatings to fuel cell membranes.

- Functional polymeric surfaces employing thio-click chemistries.

- Sports and High Performance Materials, Glassy Polymer Networks, Sustainable and Degradable Polymers, Reaction Extrusion and Polymer Processing.

- Self-assembly of stimuli-responsive block copolymers and biomimetic materials.

- Property-structure relationships in polypeptide-based micelles, (organo)gels, and liquid crystals.

- Stimuli-Responsive Polymeric Coatings; Surface/Interfacial Interactions in Organic Coatings and Film Formation; Stratification Processes in Polymeric Films.

Contact

Gordon Cannon , Ph.D.
Vice Provost for Research
118 College Drive #5116
Hattiesburg, MS 39406-0001
email: Gordon.Cannon@usm.edu
Phone: 601.266.5116
Fax: 601.266.5755
www.usm.edu

THE UNIVERSITY OF MISSISSIPPI

Capabilities in Materials

UM capabilities, expertise, and interests in materials are distributed across several academic and research units, and are being applied in several application areas.

> **Academic units** with materials capabilities including the School of Engineering (Mechanical, Chemical, Civil, and Electrical, and Geological), School of Liberal Arts (Physics, Biology, Chemistry & Biochemistry, & Geology), & School of Pharmacy (Medicinal Chemistry, Pharmacology).
>
> **Centers and institutes** with materials research, educational, and outreach capabilities include the National Center for Physical Acoustics, the Research Institute of Pharmaceutical Sciences, the Center for Wireless Communications, and the Center for Math and Science Education.
>
> **Application areas** include Energy (geological materials, solar cells, and semi-conductors, thermoelectrics, metallic hydrides, energy harvesting); Infrastructure (security, cement, and concrete); Sensors and communication systems (reconfigurable antennas, structural health monitoring, cloaking); and Healthcare (designing and characterizing materials for medical devices, nano-sensors, and nano-machines for time-dependent drug delivery).

Research capabilities and expertise include:

- Developing blast and impact resistant materials for structure protection
- Experimental characterization of composites, including electrical, thermal, and mechanical properties (including extreme environments)
- Thermal and kinetic modeling, including resign injection
- The optimization of manufacturing processes using composite materials
- Commercial-scale pultrusion capabilities, including process development and pultruded product characterization
- Optimizing material properties by modeling and engineering nano-scale structures
- Novel materials for vibrational energy harvesting
- Temperature and pressure induced critical phenomena
- Applying artificial neural networks to project expected materials properties
- Understanding the reaction of cells to external stimuli to inform design of nano-machines for improved time-dependent delivery of drugs
- Conducting simulations of nanoparticle-enhanced composites
- Designing chemical materials for solar energy conservation
- Designing nanoparticles and cost-effective materials for battery electrode materials and fuel cells
- Calculating properties of amine-containing molecules relevant to their propensity to capture CO2

- Conducting molecular dynamics simulation of CO2-carbonaceous surfaces
- Designing molecules for light harvesting
- Designing molecules for photocatalytic splitting of water
- Microbial conditioning of biomass for ethanol production
- Professional development to help secondary school teachers introduce materials science and applied engineering techniques into their classrooms

In recent years, UM researchers have authored or contributed to dozens of articles published in materials-related scientific journals, including: the *Journal of Materials Science*, *Composites*, *Computational Materials Science*, the *Journal of Reinforced Plastics and Composites*, the *Journal of Applied Polymer Sciences*, the *Journal of Polymer Composites*, *Physical Review B*, *Journal of the Acoustical Society of America,* and the *Journal of Neurosurgery*, among others.

Please direct any questions about UM Materials expertise or capabilities to one of the following:

Dr. Alice Clark
Vice Chancellor for Research and Sponsored Programs
vcrsp@olemiss.edu
662-915-7583

Mr. Jason Hale
Director of Research Resources
Office of the Vice Chancellor for Research and Sponsored Programs
jghale@olemiss.edu
662-915-3922

Dr. Joseph Gladden
Associate Professor of Physics
jgladden@olemiss.edu
662-915-7428

Nano-fabrication:

- Design and production of nanoscale devices and subsystems for battery and sensor applications.
- Reactive Ion Etching
- Metal Evaporation
- Chemical vapor Deposition (carbon nanotubes etc.)
- Sol-gel and wet chemical bottom up fabrication

Nano-Characterization Tools:

- Transmission Electron Microscopy
- Scanning Electron Microscopy
- Atomic Force Microscopy
- Xray Diffraction
- Raman Spectroscopy
- Nano-indentation Hardness Testing

Core-Laboratories:

- Nanoscale Processing and Characterization Laboratory
- Advanced Materials Science Laboratory

Computational Nanoscience:

- Fundamental first principle calculations of phenomena on the nanoscale
- Transport and optical properties of carbon nanotube-based materials
- Spectroscopy of metal nanoparticle-based biomaterials.

Student-Based Nano-Research Facility and Capabilities

- Student Laboratory for Materials Research
- Educational Scanning Tunneling Microscopy
- Educational Atomic Force Microscopy
- Xray Analysis System
- Sol-gel Preparation Stations

Contact

Wilbur L. Walters Jr.
Chair, Department of Physics, Atmospheric Sciences and Geoscience
wilbur.l.walters@jsums.edu
601-979-7012

Capabilities in Materials

MSU has taken a unique approach toward its teaming of materials science and engineering researchers. Since 1995, our faculty have organized into a University wide Materials Working Group (MWG) to promote and collaborate on research, education, and instrumentation. The MWG is a diverse, interdisciplinary group of 64 faculty representing 9 departments within 3 colleges in addition to 4 centers.

Academic units with materials capabilities include: the College of Engineering (Mechanical, Chemical, Civil, Bioengineering, and Electrical & Computer Science), College of Arts & Sciences (Chemistry, Physics & Astronomy, and Geosciences), and College of Forest Resources (Forest Products).

Centers and institutes with materials research include: The Center for Advanced Vehicular Systems (CAVS), Raspet Flight Research Laboratory, the Institute for Imaging and Analytical Technologies (I^2AT), the Energy Institute, and the Center for Computational Sciences (CCS).

Application areas include: advanced manufacturing processes, pharmaceutical processing, high temperature electronics and sensors, fatigue and fracture, bioengineering, nanomaterials, geological materials, fuel cells and batteries, computational physics, and integrated computational materials engineering.

Selected examples of research capabilities and expertise include:

- Modeling of fatigue and fracture in metallic systems.
- Experimental characterization of composites including extreme environments.
- Optimization of manufacturing processes using composite and nanomaterials.
- Development of advanced manufacturing processes with current focus on friction stir welding.
- Integrated computational materials engineering.
- Crystal plasticity and continuum model development of metals deformation.
- Modeling of plasticity across length scales.
- Synthesis of Silicon Carbide electronics and sensors for high temperature applications.
- CVD-based growth of Silicon Carbide nanowires for biomedical applications.
- Classical micromechanics modeling of nanocomposites with carbon nanofibers and interphases.
- Influence of defects on particle breakage for pharmaceuticals.
- Physics-based modeling of magnetic systems.
- Research on limestone formation and alteration for protection of water resources.
- Organic core-shell nanoparticles for color applications.
- Structure and aggregation in surface polymerized nanoparticles.
- Characterization of nanoparticles produced from wood & biomass materials.

- Synthesis of nanomaterials for property improvement.
- Materials synthesis and processing.
- Catalysis and fuel cells.

Faculty at MSU obtain funding from a wide variety of competitive government and industrial contracts and grants. Governmental funding agencies include but are not limited to: DOE, DOD, AFOSR, NASA, NSF, AFRL, ONR, and USDA.

Faculty regularly publish their research results in various scientific journals including but not limited to: Journal of Composite Materials, Metallurgical Transactions A and B, SAMPE Journal, Welding Journal, Journal of Material Science, Thin Solid Films, Materials Science and Engineering A, International Journal of Fatigue, Journal of Materials, Journal of ASTM International, Scripta Materialia, Acta Materialia, Journal of American Ceramic Society, Journal of Materials Research, Journal of Materials Processing and Manufacturing Science, Materials Letters, Nanostructured Materials, Computational Materials Science, Oxidation of Metals, Journal of the Mechanics and Physical of Solids, International Journal of Plasticity, Modeling and Simulation in Materials Science and Engineering, Crystal Growth and Design, Journal of Applied Physics, Applied Physics Letters, Physical Review B, Journal of Electronic Materials, Science, Forest Products Journal, Journal of Sedimentary Petrology, Journal of Sedimentary Research, Palaios, Carbonates & Evaporites, Applied Polymer Science, Macromolecules, Carbon, Chemistry of Materials.

Please direct any questions about MSU Materials Science & Engineering expertise or capabilities to one of the following:

Dr. David Shaw
Vice President for Research
and Economic Development
dshaw@research.msstate.edu
662-325-3570

Dr. Ray Vaughn
Associate Vice President for Research
vaughn@research.msstate.edu
662-325-3570

Dr. Lori Bruce
Associate Dean for Research
Bagley College of Engineering
bruce@bagley.msstate.edu
662-325-2270

Dr. Judy Schneider
Past Chair, MWG
Mechanical Engineering Department
schneider@me.msstate.edu
662-325-9154