Departmental Facilities and Individual Faculty Research Laboratories:

**Accelerator Laboratory**

**Director:** Dr. Lin Shao

The Accelerator Laboratory is one of the largest university ion irradiation facilities in the U.S. A total of five accelerators are able to deliver virtually all ions in the elemental table with ion energy from a few hundred eV to a few MeVs. The lab provides unique capabilities to perform accelerator based irradiation studies on various nuclear materials. The Accelerator Laboratory is also very active in multidisciplinary research, including fundamental ion solid interactions, accelerator based ion beam mixing, ion beam assisted film deposition, ion doping, Rutherford backscattering spectrometry, elastic recoil detection analysis, nuclear reaction analysis, and particle induced X-ray emission analysis.

The mission of the Laboratory is to provide an open facility designed to support research and teaching efforts in materials science. The Accelerator Laboratory has played an active role in building an interdisciplinary research program at Texas A&M University. The facilities have provided over five hundred hours of irradiation annually for various collaborative research projects with industry and national laboratories. The facilities provide hands-on training for students across the campus. Once students pass the training and on-site tests, they are qualified as operators to conduct their own research projects using the accelerators.

The key facilities in the Accelerator Laboratory include: a 10 kV Ion Accelerator (with a gas ion source); a 150 kV Ion Accelerator (with a universal ion source); a 200 kV Ion Accelerator (with a universal ion source); a 1 MV Ionex Tandetron Accelerator (with a RF Plasma Source and a SNICS source); a 1.7 MV Ionex Tandetron Accelerator (with a RF Plasma Source and a SNICS source); a high temperature vacuum furnace; a high temperature gas furnace; a four-point-probe resistivity measurement; and various heating and cooling systems for ion irradiations at different temperatures.

All five accelerators provide mass-analyzed ion beams of most of the elements of the periodic table. 1 MV and 1.7 MV ion accelerators are modified General Ionex Tandetron accelerators. Each of them has its own scanning systems, electrostatic deflectors, an injector and an analyzing magnet. The general purpose chamber has been equipped with numerous unique designs for various ion beam applications.
**AGN-201M Reactor Laboratory**

**Contact:** Jerry Newhouse

The AGN reactor has a thermal power rating of 5W. The reactor utilizes a homogeneously mixed polyethylene and UO₂ plate type fuel. The fuel is surrounded by graphite and is contained within a pressure tight vessel fabricated from aluminum. Natural convection maintains the core temperature relatively stable by removing heat that is generated being lost to the water surrounding the core. The reactor is controlled by four fueled control rods that are inserted into the core to maintain control of the nuclear reaction.

**Center for Large-Scale Scientific Simulations (CLASS)**

**Director:** Dr. Jim Morel

One objective of the Center for Large-Scale Scientific Simulations (CLASS) is to advance the state of the art in large-scale scientific simulations. This means developing numerical methods and computational strategies that enable more efficient solutions of larger problems on the latest computer platforms. The second objective is to lead the development of educational programs whose participants will be exceptionally well qualified for careers in scientific simulation. CLASS is working toward this objective by bringing together key faculty members from several departments (including Mathematics, Computer Science, and Nuclear Engineering) and key national-lab practitioners to collaboratively design graduate programs that will provide the broad range of skills and knowledge that are needed by tomorrow's experts in scientific simulation.

**Fuel Cycle and Materials Laboratory (FCML)**

**Director:** Dr. Sean McDeavitt

The FCML has been dedicated to innovative research, training and services in nuclear fuel management, as well as fuel fabrication and materials science. The FCML was established at Texas A&M University in 2006 with an intent to locate alternative and more efficient methods within the nuclear fuel cycle in order to permit safe, protected, commercial, and maintainable development of nuclear energy while lessening risks linked to proliferation effects.

The Fuel Cycle and Materials Laboratory (FCML) was established to study current issues in the nuclear fuel cycle, including materials and chemical processing, advanced fuels and materials, and waste immobilization. Equipment in FCML includes high temperature furnaces, two inert atmosphere gloved boxes, and a 90-ton hydraulic press. These may be configured for casting, instrumented sintering, cold or hot pressing, and hot extrusion. Further, the laboratory is equipped and has been approved for the handling, testing and characterization of radioactive materials. Currently funded projects from the US Department of Energy include materials processing activities to develop advanced nuclear fuels for burning transuranic radionuclides and radioactive waste forms for isolating fission products.

**Lab Equipment List**

A. Central Argon, Air
B. IONEX 0-G-2502 Sample Glovebox
C. Polisher-Buehler Minimet 1000
D. Digital Optical Microscope-HiRox KH – 1300 with a MX – 5040SZ Lens
E. Atlas Auto 40T Hydraulic Press
F. Ultra High Temperature/Vacuum Materials Research Furnace
G. M1-10A Portable Water Chiller
H. HEPA Filter
I. Diamond Saw: Leco VC-50
J. Hot Isostatic Press: IPS Eagle 6
K. Laser Flash Analysis-Netzsch LFA 447 NanoFlash
L. Differential Scanning Calorimetry-STA 409 PC
M. Controlled Atmosphere Furnace-Deltech DT-28-STBL-B-E2404
N. Hydraulic Press-Enerpac IP-Series
O. Heat Treatment Furnace-Lindberg/Blue 818
P. Small Glove Box

**Institute for National Security Education & Research (INSER)**

**Director:** Dr. Marvin Adams

INSER develops and implements graduate-level education programs targeted at national security professionals. For example, it currently works with Texas A&M's Bush School of Government and Public Service to provide a Graduate Certificate program in National Security Affairs to selected employees from Lawrence Livermore National Laboratory. INSER also organizes and implements multidisciplinary research and development programs that are relevant to national security. Current programs include those targeted at Nuclear Nonproliferation; Scientific Simulation relevant to national security; and Homeland and International Security.

**Interphase Transport Phenomena Laboratory (ITP)**

**Contact:** Dr. Cable Kurwitz

The ITP Laboratory conducts research in the area of interfacial heat, mass and momentum transport. The ITP group has worked in the areas of modeling and measurement of zero gravity multiphase flow systems including the development of technologies for implementing in zero and reduced gravities. Laboratory experiments have flown on more than 50 reduced gravity aircraft flight campaigns amassing over 10,000 parabolas of experience. In addition, the laboratory has had hardware developed and flown on the space shuttle, space station, and suborbital vehicles. The laboratory was part of a multiagency effort to test a loop heat pipe on orbit as part of STS-87. Currently, the laboratory is working on a number of advanced thermal and fluid management technologies for NASA and industry.

**Ion Beam Laboratory**

As one of the largest ion irradiation facilities in the US, the Ions & Materials Facility was built and designed to use as a platform for interdisciplinary research and teaching. A total of five accelerators are available to produce beams of virtually any ion species in the energy region of a few hundred eV up to a few MeV. This gains us flexibility to systematic ion irradiation studies under various conditions. Due to the need of large space for these giant machines, the facility is split into two labs, one is located on campus and another a few miles away from the campus. By combining the ion irradiation capability from our lab (ions of sub keV to MeVs) with that from **Cyclotron Institute** (ions of 100 MeVs) and from **Nuclear Science Center** (neutrons and gamma
rays), we can offer wide-ranging capabilities for the production and investigation of radiation effects in materials.

**Laser Diagnostics Multiphase Flow Laboratory**
**Director:** Dr. Yassin Hassan
The mission of the laboratory is to investigate the complex, multiphase flow of multiscale, multi-physics flow phenomena using non-intrusive global field measurement techniques. The laboratory provides the ability to use state-of-the-art particle image velocimetry techniques to study these flows. The laboratory is equipped with fast-pulsed, high-energy lasers and fast high-resolution cameras. Data are analyzed using in-house developed tracking, imaging and pattern recognition routines. The combination of instantaneous measurements of full-fields of velocity and laser-induced temperature measurements enables a multitude of interesting studies of single and multiphase flows.

**Micro-Beam Cell Irradiation Facility**
**Contact:** Dr. John Ford
The microbeam cell irradiation facility provides specialized irradiation capabilities needed to implement radiation biology experiments to understand the cellular and molecular mechanisms controlling the risk of long term health effects related to low doses of ionizing radiation. Radiation sources include 250 keV x ray machine, 80 keV electron microbeam, and 2 MeV tandem electrostatic accelerator with single particle microbeam capability. The microbeam facilities can reproduce most of the range of charged particles that are found in environmental and industrial settings, and are designed to facilitate study of effects in bystander cells and other biological phenomena that are found at low doses.

**Nuclear Heat Transfer Systems Laboratory**
**Director:** Dr. Karen Vierow-Kirkland
The Nuclear Heat Transfer Systems Lab was established with the initial goals of investigating condensation heat transfer mechanisms, experimentally and analytically investigating new reactor designs and safety systems, and advancing the state-of-the-art in reactor safety analysis. Department of Energy projects and support from Japanese nuclear utilities have been supporting several M.S. and Ph.D. students to perform experimental investigations of passive heat removal systems in advanced light-water reactors and to quantify uncertainties in modeling of Gen IV reactors. These and other projects from the US Nuclear Regulatory Commission and Sandia National Laboratories have enabled the lab to construct thermal hydraulic facilities for testing of advanced safety system concepts, derive theoretical formulations for condensation heat removal in the presence of a non-condensable gas and advance severe accident analysis methodologies. The lab is equipped with a 150-kW steam supply, a high speed camera, extensive thermal hydraulic instrumentation and a state-of-the-art data acquisition system. New efforts focus on developing analysis methods for high-temperature, gas-cooled reactors, improving best estimate analysis with Probabilistic Risk Analysis methodologies and development of detectors for Special Nuclear Materials.
**Nuclear Power Institute (NPI)**

**Director:** Dr. Kenneth Peddicord

The Nuclear Power Institute is a statewide partnership led by the Texas Engineering Experiment Station (TEES) and headquartered at Texas A&M University. The partnership includes universities, community colleges, the nuclear power industry, state agencies and local organizations. The objective of NPI is to develop the necessary workforce for the new nuclear power plants that will be developed in Texas and to sustain a vibrant new, clean industry in the State.

**Nuclear Science Center**

**Director:** Dr. Sean McDeavitt

This facility has a one-megawatt TRIGA swimming pool reactor that can be pulsed and a variety of other features including experimental laboratories, a large irradiation cell, beam ports, a thermal column and a pneumatic "rabbit" system. One of the best-equipped facilities of its type in the country, the facility is used in our laboratory courses as well as our research program.

The goal of the Nuclear Science Center is to improve the health, well-being and environment of mankind through the application of nuclear technology. The Nuclear Science Center, located near the southwest side of Easterwood Airport, houses a 1 MW research reactor and associated research facilities. The center provides services to researchers and/or faculty from Texas A&M University, other colleges and universities, government agencies and private industry. The center is recognized primarily for providing radioisotopes and other nuclear irradiation services for research, academic, medical and industrial applications and as a teaching and nuclear training facility.

We are a multidisciplinary research and education center supporting basic and applied research in nuclear-related fields of science and technology and providing educational opportunities for students in these fields as a service to the public and The Texas A&M University System. We also provide services to commercial ventures and industry requiring irradiation, training, or isotope production services.

Our reactor is designed for optimal irradiation of various types of samples and is used to produce various radioisotopes for industry, medical and academic users. We are nationally recognized for our neutron activation analysis services to many research and academic institutions in the United States.

We support the Department of Nuclear Engineering at Texas A&M University, the largest nuclear engineering program in the country. We serve about 80 nuclear engineering students each year through our teaching and research activities.

The goal of the Nuclear Science Center is to improve the health, well-being and environment of mankind through the application of nuclear technology. The Nuclear Science Center houses a 1 MW research reactor and associated research facilities. The center provides services to researchers and/or faculty from Texas A&M University, other colleges and universities, government agencies and private industry. The center is recognized primarily for providing radioisotopes and other nuclear irradiation services for research, academic, medical and industrial applications and as a teaching and nuclear training facility. **Products and Services**

**Facilities and Equipment**

- **Irradiation Cell**
- In-core irradiation devices
- Radiochemistry lab
- Neutron activation analysis and counting lab
- Delayed neutron counting system
- Radiation protection and instrumentation
- Nuclear electronics and machine shops

**Nuclear Security Science & Policy Institute (NSSPI)**

**Director:** Sunil Chirayath

The Nuclear Security Science and Policy (NSSPI) Institute is a joint TEES/TAMU center housed in the Nuclear Engineering Department and in collaboration with the George Bush School of Government and Public Service. The mission of NSSPI is to work collaboratively with national laboratories and other partners to develop and apply science and technology to detect, prevent, and reverse the proliferation of nuclear and radiological weapons and guard against nuclear terrorism; educate the next generation of leaders in the field of nuclear security sciences; and to study the policy implications of deploying new technologies. NSSPI provides research, education, and support in the area of nuclear security especially with respect to the interface between policy and technology.

**Radiation Detection Measurement Laboratory**

The radiation detection measurement laboratory maintains a wide variety of instrumentation that is employed to study radiation and radioactive decay. This laboratory is used to educate students on the fundamentals of radiation detection and allows them to explore current advances in the field. To demonstrate detector components, Nuclear Instrument Modules (NIM) are maintained and used to operate Geiger-Mueller tubes, gas-flow proportional counters, alpha-spectrometers, gamma detectors and neutron detectors. For more advanced laboratories, students use digital electronic based systems to study gamma spectroscopy, coincident radiation, neutron detection and neutron multiplicity. To accomplish this work, the Nuclear Engineering Department maintains high-purity germanium (HPGe) workstations, hand-held radiation identification systems as well as He-3 and BF-3 tubes for neutron detection. The laboratory is used both in the educational and research programs for the department.

**Tandem Accelerator Laboratory**

**Director:** Dr. Leslie Braby

A 2 MeV Pelletron accelerator provides charged particle beams for radiation biology and dosimetry studies. Beam lines for single particle microbeam biology studies and for charged particle track structure studies are available. The accelerator provides particles in the energy range typical of proton recoils from neutron irradiation and alpha particles from radioactive sources.
Multi-User TAMU Facilities used by Mechanical Engineering Faculty:

Supercomputing Facilities:

**TAMU High Performance Research Computing**

This resource for research and discovery has four available clusters for faculty research:

1. Ada is a 17,340-core IBM/Lenovo commodity cluster with nodes based mostly on Intel's 64-bit 10-core IvyBridge processors. In addition to the 852 compute nodes, there are 8 login nodes, each with 256 GB of memory and GPUs or Phi coprocessors per node.

2. Crick is a 368-core IBM Power7+ BigData cluster with nodes based on IBM's 64-bit 16-core Power7+ processors. Included in the 23 nodes are 1 BigSQL node with 256GB of memory per node and 14TB (raw) of storage and 22 data nodes with 14TB (raw) storage for GPFS-FPO and local caching. Crick is primarily used for big data analytics. In addition to these nodes are 2 login nodes with 128GB of memory per node.

3. Curie is an 768-core IBM Power7+ cluster with nodes based on IBM's 64-bit 16-core Power7+ processors. In addition to the 48 nodes are 2 login nodes with 256GB of memory per node. Curie's file system and batch scheduler are shared with Ada cluster.

4. LoneStar5 is the latest cluster hosted by the Texas Advanced computing Center. Jointly funded by the University of Texas System, Texas A&M University and Texas Tech University, it provides additional resources to TAMU researchers. LoneStar5 has: 252 Cray XC40 compute nodes, each with two 12-core Intel® Xeon® processing cores for a total of 30,048 compute cores; 2 large memory compute nodes, each with 1TB memory; 8 large memory compute nodes, each with 512GB memory; 16 Nodes with NVIDIA K-40 GPUs; 5 Petabyte DataDirect Networks storage system; and Cray-developed Aries interconnect.

The HPRC group provides its users with access to several specially configured "HPRC Lab" Linux workstations at two separate locations on the TAMU campus, and can assist with: debugging, code optimization and parallelization, batch processing, and collaborative advanced program support.

**Texas Advanced Computing Center (TACC)**

The Texas Advanced Computing Center (TACC) designs and operates some of the world's most powerful computing resources. The center's mission is to enable discoveries that advance science and society through the application of advanced computing technologies. Through this center TAMU faculty have access to multiple supercomputers, including:

- **Stampede** - has 6,400 Dell C8220 compute nodes are housed in 160 racks; each node has two Intel E5 8-core (Sandy Bridge) processors and an Intel Xeon Phi 61-core (Knights Corner) coprocessor. Stampede is a multi-use, cyberinfrastructure resource offering large memory, large data transfer, and graphic processor unit (GPU) capabilities for data-intensive, accelerated or visualization computing. To this end, there are also 16 large-memory nodes with 1 terabyte (TB) memory, as well as 128 compute nodes with NVIDIA Kepler K20 GPUs. All components are integrated with an InfiniBand FDR network of Mellanox switches to deliver extreme scalability and high-speed networking.

- **Lonestar**
• 1252 Cray XC40 compute nodes, each with two 12-core Intel® Xeon® processing cores for a total of 30,048 compute cores
• 2 large memory compute nodes, each with 1TB memory
• 8 large memory compute nodes, each with 512GB memory
• 16 Nodes with NVIDIA K-40 GPUs
• 5 Petabyte DataDirect Networks storage system
• Cray-developed Aries interconnect

Wrangler:
System Features
• Geographically replicated, high performance data storage (10PB each site)
• Large scale flash storage tier for analytics with bandwidth of 1TB/s and 250M IOPS (6x faster than Stampede)
• More than 3,000 embedded processor cores for data analysis
• Flexible support for a wide range of data workflows, including those using Hadoop and databases.
• Integration with Globus Online services for rapid and reliable data transfer and sharing.
• A fully scalable design that can grow with the amount of users and as data applications grow.

Wrangler Subsystems:
• A 10PB storage system
• A set of 120 Intel Haswell-based servers for data access and embedded analytics
• A high-speed global object store made from NAND Flash

Other Multi-User Facilities:

**Center for Chemical Characterization and Analysis (CCCA)**

**Director:** Dr. Emile Schweikert, Department of Chemistry

**Nuclear Magnetic Resonance (NMR) Facility** - The NMR Facility includes 10 superconducting spectrometer magnet systems, 4 LINUX workstations dedicated to data processing, and 3 full time staff to support them with maintenance, user training, and spectroscopic service. Although this facility is physically housed within the Chemistry Department, it provides services to the entire campus community.

**X-Ray Diffraction Laboratory** - The lab maintains 3 Micro-focus IuS sources, a Venture CMOS, QUEST CMOS, three Bruker single-crystal APEXii CCD Diffractometers, 1 Bruker GADDS/Histar diffractometer, and 3 Bruker powder diffractometers. The X-ray Diffraction Laboratory is staffed by two full-time Ph.D. level scientists.

**Laboratory for Biological Mass Spectrometry – Chemistry Mass Spectrometry Facility** – The services available include analyses of compounds ranging from small organic molecules to macromolecules including proteins, oligonucleotides, polymers and dendrimers. Instruments available include: Applied Biosystems PE SCIEX QSTAR; Thermo Scientific DSQ II GCMS; and Thermo Scientific LCQ-DECA

**Center for Mass Spectrometry** - is dedicated to providing cutting-edge technology and expertise for the characterization of molecules to fulfill the needs of researchers at TAMU. Mass spectrometry (MS) plays an increasingly important role in molecular level research, and it is central to ‘omics’ research, i.e., petroleomics, proteomics,
metabolomics, lipidomics, glycomics, etc and the CMS provides expert staff with modern instrumentation to complete these tasks. Instruments available include: Thermo Scientific Fusion; Bruker 9.4T FT-ICR MS; MDS-Sciex 4000 Qtrap; and Applied Biosystems 4800+ MALDI TOF/TOF MS.

Elemental Analysis - The laboratory provides research support in the area of elemental and trace analysis as well as service analyses to TAMU users, other university and government agencies and private industry. It is unique in that it features fast neutron activation analysis (FNAA) capabilities in addition to thermal instrumental neutron activation (INAA) using the University's Nuclear Science Center 1 MW TRIGA research reactor. In addition, the laboratory has recently added inductively-coupled plasma - mass spectrometry to its stable of facilities. The ICP-MS has been fitted with both conventional sample introduction hardware for solution work as well as a 213 nm laser ablation system for studying solids and surfaces.

Cyclotron Institute
Director: Dr. Sherry Yennello
The Cyclotron Institute is a major accelerator facility, jointly funded by the State of Texas and the Department of Energy that carries out a program of basic research and education in both nuclear physics and nuclear chemistry. This program includes experimental and theoretical work in nuclear structure, nuclear astrophysics, fundamental interactions, nuclear dynamics, and atomic physics. Recent upgrades will significantly extend the Institute's research capabilities as a stable beam facility with moderate rare ion beams. In addition, the Institute serves as one of the primary facilities in the country for the testing of space-bound microelectronic devices. Research is conducted on a wide variety of modern experimental equipment using accelerated ions from two cyclotrons - a newly refurbished K150 cyclotron and a superconducting K500 cyclotron.

The Texas A&M Cyclotron Institute includes K500 Cyclotron, ERC Ion Sources, MARS, Big Sol, MDM Spectrometer, NIMROD, Precision On-Line Decay Facility, K150 Cyclotron, Light Ion Guide, Heavy Ion Guide, Negative Ion Source, CB-ECRIS, and Radiation Effects Facility.

Energy Institute
The Texas A&M Energy Institute interdisciplinary research program focuses on the interacting themes of:

a. Fossil and Non-Fossil based Technologies for Energy;
b. Materials, Catalysis, and Separations for Energy;
c. Multi-scale Energy Systems Engineering; and

The four interconnected themes are further classified into (10) research areas, and (65) research topics. To enhance the synergy among different disciplines, the Texas A&M Energy Institute introduces annual multi-PI proposal calls and provides seed and matching funds for competitively selected group projects.

Texas A&M University is home to world-class research facilities which include the newly constructed Giesecke Engineering Research Building (GERB). The GERB is home to multidisciplinary researchers and faculty from the over 240 faculty affiliated with the Texas A&M Energy Institute. In the GERB, three focus areas are housed; Nanotechnology, Materials Science, and Computational Science. Researchers from the departments of Chemical
Engineering, Electrical Engineering, and Mechanical Engineering cross-pollinate to lead to cutting-edge, interdisciplinary breakthroughs.

**Institute for Scientific Computation**

**Director:** Dr. Yalchin Efendiev

The ISC is a multidisciplinary research center devoted to designing, analyzing, and implementing innovative computational tools that advance scientific engineering research and education. ISC researchers include internationally recognized Texas A&M faculty members devoted to collaborating on major national and global research efforts with other universities, industrial partners, and the government. The ISC also serves as an excellent training ground for students, both graduate and undergraduate, and postdoctoral scholars in a variety of academic disciplines within scientific computing technologies.

**Immersive Visualization Center**

The Immersive Visualization Center provides the latest in advanced visualization capabilities to researchers at Texas A&M University. Based on a semi-rigid, rear projected, curved screen, the IVC facilitates the imaging of very large datasets from a diverse set of disciplines. Geophysics, life and physical sciences, engineering, and architecture are all able to gain a better understanding of their research by taming the complexity of their data through visualization.

This particular configuration is the first such installation in the world. The screen was constructed by SEOS and is driven by a custom-built SuperMicro workstation from R Associates running Linux. The IVC is housed in space provided by the Department of Geology and Geophysics and is operated by the Institute for Scientific Computation.

**Laboratory for Molecular Simulation**

The Laboratory for Molecular Simulation (LMS) brings molecular modeling and computational chemistry closer to the experimental scientist by offering training to both new and advanced users. Advanced modeling software is available for researchers at Texas A&M University to perform quantum calculations on small molecular or solid systems and molecular mechanics/dynamics modeling for large systems such as proteins, DNA, nanomolecules, polymers, solids, and liquids. The LMS also provides support for faculty that wish to incorporate molecular modeling in their course material.

Resources available at the LMS include:

**WORKSHOPS** - The LMS offers, free of charge, three types of workshops throughout the year:

1) Linux, 2) Molecular Modelling, and 3) Quantum Mechanics Short Course. For more information please see the workshops link to the left. Most of the programs available through the LMS are only available on Linux based machines, therefore, the Linux workshop is a prerequisite for all other workshops.

**HARDWARE** - The LMS has 20 SUN Ultra 20 workstations, 1 dual processor SGI Octane, 3 SGI R12000 O2's, and 4 Power Mac G5's in the computer lab in room 2109 chemistry. To obtain an account you must complete the Linux workshop or have a VERY strong background in Linux or UNIX. For information or an account on one of the LMS computers, please contact Lisa M. Pérez.

**SOFTWARE** - The LMS has a wide variety of molecular modelling software available. Below is a list of each program with a very brief description of it's purpose. For detailed information
please visit the program links to the left. If you are interested in obtaining access to this software, want to test a program/module that we currently do not have a license for, or simply have questions about the software, please contact Lisa M. Pérez.

**ADF/ADF-BAND** - ADF Package, by SCM is package is software for first-principles electronic structure calculations. ADF is used by academic and industrial researchers worldwide in such diverse fields as pharmacochemistry and materials science. (Linux IA64)

**AMBER** - AMBER, by David Case at The Scripps Research Institute and collaborators, is the collective name for a suite of programs that allow users to carry out molecular dynamics simulations, particularly on biomolecules. (IRIX, AIX, Linux, Windows, and MacOS X)

**AOMix** - AOMix is a user-friendly Windows software package for molecular orbital (MO) analysis and spectra simulation from results obtained from the following software packages: ADF, GAMESS, Gaussian, HyperChem, Jaguar, MOPAC, Q-Chem, Spartan, and ZINDO. (Windows)

**CHARMm** - CHARMm (Chemistry at HARvard Macromolecular Mechanics) is a highly regarded and widely used simulation package for small organic molecules, proteins, DNA, and RNA, which combines standard minimization and dynamics capabilities with expert features including normal mode calculations, and correlation analysis. (IRIX, Linux, and Windows)

**Dalton** - Dalton QCP is a powerful quantum chemistry program for the calculation of molecular properties with SCF, MP2, MCSCF or CC wave functions. (emphasis on magnetic and electric properties) (IRIX and Linux)

**Discovery Studio** - A user-friendly graphical molecular modelling program developed by Accelrys Inc., that incorporates a variety of useful molecular modelling codes specifically designed for biological systems. (Windows and Linux)

**Gaussian 03 (G03)** - A suite of programs to perform semi-empirical and *ab initio* molecular orbital calculations on Linux/UNIX based machines (IRIX, AIX, Linux, MacOS X, and Windows)

**GaussView** - The GUI interface to Guassian 03. This program is used to assist the user in setting up calculations, and to visualize results (optimized geometries, molecular orbitals, potential surfaces, vibrational modes, etc.) (IRIX, AIX, Linux, and Windows)

**Materials Studio** - A Windows based program designed by Accelrys Inc. for the material sciences. The newest developements of the materials science modules available in cerius2 will only be found in materials studio. Many of the internal programs also run on Linux. (Windows and Linux)

**Molden** - A graphical program that will allow users of a wide variety of molecular modelling codes (including G98) to visualize their results. (IRIX, AIX, Windows, MacOS X and Linux)

**MOLEOnline** - MOLEOnline provides an interactive web-based tool to found and analyze molecular channels, tunnels and pores. (on-line)

**MOLPRO** - A complete system of *ab initio* programs for molecular electronic structure calculations with an emphasis is on highly accurate computations, with extensive treatment of the electron correlation problem through the multiconfiguration-reference CI, coupled cluster and associated methods. (IRIX, AIX, and Linux)
**Q-Chem** - A modern ab initio, electronic structure program package, capable of performing first principles calculations on the ground and excited states of molecules. (IRIX)

**Quanta** - A graphical molecular modelling program that has historically been used for life science calculations (CHARMM) and X-ray crystallography, but is currently developed with advanced tools for macromolecular X-ray crystallographers. (IRIX and Linux)

**SPOCK** - A full-featured molecular graphics program developed by Dr. Jon A Christopher while in the lab of Thomas O. Baldwin of the Department of Biochemistry & Biophysics at Texas A&M University. Spock has been designed from the ground up to be powerful, flexible and most of all, easy to use. (IRIX)

**TINKER** - The TINKER molecular modeling software is a complete and general package for molecular mechanics and dynamics, with some special features for biopolymers. TINKER has the ability to use any of several common parameter sets, such as AMBER94/96, CHARMM27, MM2(1991), MM3(2000), OPLS-AA and OPLS-UA. (IRIX, Linux, and Windows)

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**Materials Characterization Facility**

The Materials Characterization Facility (MCF) at Texas A&M University is a multi-user facility located in the Frederick E. Giesecke Engineering Research Building (GERB) housing the fabrication and characterization instrumentation essential for the development, understanding, and study of new materials and devices. Specific instrumentation available include:

**Electron Microscopy:**
- Field Emission-Scanning Electron Microscope (FE-SEM) (JEOL JSM-7500F),
- Lyra Focused Ion Beam-Scanning Electron Microscope (FIB-SEM) with an EDS Microanalysis System,
- Fera Focused Ion Beam-Scanning Electron Microscope (FIB-SEM) with EBSD and Integrated Time-of-Flight Mass Spectrometer (ToF-SIMS), and
- Electron microprobe with Wavelength Dispersive Spectroscopy (WDS)

**Thermal and Electrical Analysis**
- **Thermal mechanical analysis (TMA)**
- **Dynamic mechanical analysis (DMA)**
- **Differential scanning calorimetry (DSC)**
- **Dielectric spectroscopy**
- **Hot Disc thermal conductivity analysis**

**Surface Analysis**
- **X-ray Photoelectron Spectroscopy (XPS)/Ultraviolet Photoelectron Spectroscopy (UPS)**
- **MultiMode Atomic Force Microscope (AFM)**
- **Nanoindenter**
- **Dip pen nanolithography**
- **Imaging ellipsometer**
- ** Cameca ion microprobe**
- **Icon Atomic Force Microscope (AFM)**

**Fabrication**
- **Electron beam deposition chamber**
Spectroscopy and Microscopy

- Spectrofluorometer
- UV-Vis-NIR spectrophotometer
- Raman confocal microscope
- Fourier Transform Infrared (FTIR) spectrometer
- Fluorescent confocal microscope

**Microscopy & Imaging Center (MIC)**

The mission of the Microscopy & Imaging Center (MIC) is to provide current and emerging technologies for teaching and research involving microscopy and imaging in Life and Physical Sciences on the Texas A&M campus and beyond, training and support services for microscopy, sample preparation, in situ elemental/molecular analyses, as well as digital image analysis and processing. This facility promotes cutting edge research in basic and applied sciences through research and development activities, as well as quality training and education through individual training, short courses and formal courses that can be taken for credit.

Instruments available at the MIC include:

- **Light Microscopy**
  - Zeiss Axiophot
  - Olympus FV1000 confocal microscope
  - Multiphoton non-linear optical microscope
  - Deconvolution
  - Nikon Stereo Photo Microscope

- **Scanning Electron Microscopy**
  - FEI Quanta 600 FE-SEM
  - Tescan Vega3 SEM
  - Zyvex S100 Nanomanipulator

- **Transmission Electron Microscopy**
  - FEI Tecnai G2 F20 FE Cryo-TEM
  - FEI Tecnai G2 F20 ST FE-TEM - Materials
  - JEOL 1200 EX TEM
  - JEOL JEM-2010 TEM
  - Analog & Digital Image Analysis
  - Ancillary Equipment

- **Correlative Light and Electron Cryo-Microscopy**
  - FEI cryo-fluorescence stage on the Olympus microscope

**National Center for Electron Beam Food Research**

**Director:** Dr. Suresh Pillai

Researchers in the National Center for Electron Beam Food Research, which has been recently designated as a National Research Center, use high- and low-energy electron beams to reduce the number of bacteria and other pathogens in and on food and other materials. The work is primarily directed at spontaneous, food-borne illness but is also relevant to bioterrorism issues.

**Texas A&M Engineering Extension Service (TEEX) Disaster City**
Located in College Station, Texas, this 52-acre training facility is situated adjacent to the TEEX Brayton Fire Training Field and delivers the full array of skills and techniques needed by today's emergency response professionals. The mock community features full-scale, collapsible structures designed to simulate various levels of disaster and wreckage which can be customized for the specific training needs of any group. Emergency responders from across the globe venture to Disaster City for search and rescue training and exercises. First responder training facilities include:

- Building Collapse
- Rubble Pile
- Technical Skills Training Area
- Transportation Disaster Training Area
- Government Complex - Project 133

**Facilities from other TAMU Departments used by Mechanical Engineering Faculty:**

**Aerosol Technology Laboratory**

**Director:** Dr. Yassin Hassan, Department of Mechanical Engineering

The Aerosol Technology Laboratory is an independent University research laboratory at the Department of Mechanical Engineering at Texas A&M University that was established under the direction of Dr. Andrew R. McFarland, Wyatt Professor of Mechanical Engineering, and has been serving for over thirty-five years as a center for aerosol research for both private and public sector interests.

Capabilities of the Aerosol Technology Laboratory include: Static bench-top testing of aerosol devices with inert monodisperse aerosol (liquid or solid particles with imbedded fluorescent tracer) as well as with non-pathogenic bacteria spores; fluorometric analysis, and imaging of test aerosol particles; culturing of bacteria spores for quantitative analysis; and wind-tunnel testing of aerosol sampling equipment with either inert aerosol particles or non-pathogenic bacteria spores. Specifically the ATL has facilities for:

**Aerosol Sampling**

- Wetted-Wall Cyclone Sampling Systems
  - Three autonomous scaled systems - 100 L/min, 400 L/min, 1250 L/min
  - Concentration Factor ~10^6
  - Cutpoint ~1µm AD
  - Low Cut Point (LCP) <500 nm AD

**Aerosol Concentration**

- Linear Slot Virtual Impactor
  - Cutpoint 1.1 µm AD
- Circumferential Slot Virtual Impactor
  - Cutpoint 2.2 µm AD

**Particle Tracking**

- Particle Detachment and Resuspension
- Particle Tracking Velocimetry
• Electrostatic Sprayer Deposition Software
  • For evaluating the penetration of aerosol through sampling systems
  • Sampling with shrouded probes
  • Flow splitters in transport systems

Biosensors
  Ion Flux Based Biosensing
  • The “injection-leakage” phenomenon
  • Sensing of Phage Triggered Ion Cascades (SEPTIC)
  • Detects fluctuations in microscopic electrical field
  Odor-Based Biosensing
  • Fold sensor systems distinguish between different odor sources
  • Identify and quantitate bacteria and fungi within complex samples

Corrosion and Biofilms
  • Different alloys
  • Different corrosion types
  • Extensive biofilm on surfaces
  • Novel, efficient biocide

**Equal Channel Angular Extrusion Laboratory**
**Contact:** Dr. Hartwig, Department of Materials Science and Engineering
The Equal Channel Angular Extrusion (ECAE) process was invented in the former Soviet Union by Vladimir Segal in 1977. Dr. Segal himself worked as an associate in the TAMU ECAE lab from 1992 to 1995. Researchers in the TAMU Deformation Processing Laboratory have been conducting research on the ECAE process since 1992. ECAE is an innovative process capable of producing uniform plastic deformation in a variety of materials without causing significant change in geometric shape or cross section.

**Fluctuation and Noise Exploitation Laboratory (FNEL)**
**Director:** Dr. Laszlo Kish, Department of Electrical and Computer Engineering
This researchers in this laboratory study New concepts, theory, simulations or experiments about various applications of fluctuations and noise, including:
  • Various aspects of unconditionally secure data communications,
  • Various aspects of noise-based logic and computing schemes,
  • Fluctuation-enhanced sensing, (chemical and/or biological); etc.

**Machine Shop in the Department of Mechanical Engineering**
The Department of Mechanical Engineering’s machine shop includes manual lathes, manual mills, vertical and horizontal band saws and welding equipment. It features a HAAS CNC TL-2 lathe, HAAS CNC SL-10 lathe and a HAAS CNC Mini Mill.
  We are capable of manufacturing just about anything that you need, and we offer consultation if you have any questions about how or if your design can be manufactured.
**Surface Science Laboratory**
**Contact:** Dr. Hong Liang, Department of Mechanical Engineering
The primary focus of our research is in the broad area of surface and interface science and engineering. This interdisciplinary area is in the frontier of science and has many important engineering applications. Current topics include, development of methodology to characterize and understand chemical, mechanical, physical, and tribological properties of surfaces and interfaces of materials in different states: solid, liquid, and vapor; development of processes to synthesize nanoparticles, nanostructured bulk materials, and surface coatings with multi-properties; and development of nanomanufacturing processes to fabricate nanostructures, nanodevices, sensors, and hybrid (including cyborg) systems. Labs include:

- Surface Science Laboratory
- Biomaterials Laboratory
- Nanomaterials Processing and Atomic Imaging Laboratory
- Tribology in Extreme Environments Laboratory

**Turbomachinery Laboratory**
**Director:** Dr. Dara Childs, Department of Mechanical Engineering
The Turbomachinery Laboratory conducts basic and applied research into important problems of reliability and performance of turbomachinery — rotating machinery that extracts or adds energy to fluids. That’s everything from classic Dutch windmills to the space shuttle’s main engine turbopumps and compressors that move natural gas through the distribution system.

The Turbomachinery Laboratory provides continuing education opportunities to users of industrial turbomachinery and pumping systems at the annual International Pump Users Symposium and Turbomachinery Symposium.

We also offer a number of intensive Short Courses throughout the year on varying topics relevant to today’s professionals in the turbomachinery and pumping industries.

Through these activities, the Turbomachinery Laboratory continues Texas A&M’s land-grant charter tradition of education, research and service.

The Turbomachinery Laboratory sponsors two large industrial symposia to provide continuing education opportunities to users of industrial turbomachinery, and to generate profits to foster and support graduate and undergraduate education in turbomachinery.

The Turbomachinery Laboratory provides an opportunity for collaborative research among faculty members throughout the college in the area of turbomachinery.

**Williams Radiogenic Isotope Geosciences Laboratory**
**Director:** Luz Maria Romero, College of Geosciences
The R. Ken Williams '45 Radiogenic Isotope Geosciences Laboratory allows College of Geosciences faculty and students to perform interdisciplinary research in marine geology, global tectonics, geochronology, and environmental and climate change issues. Equipment available in this lab includes:

- **Triton Plus Thermal Ionization Mass Spectrometer (TIMS)** - The TIMS system is ideal for the high-precision analysis of isotope ratios of Earth material, typically used for dating and tracing purposes.
• **High-resolution Inductively Coupled Plasma Mass Spectrometer Element XR** - The High-Resolution Element XR is capable of measuring the concentrations of metals and non-metals within a high dynamic range, i.e., concentrations as low as parts per trillion (ppt) to as high as parts per thousand (permil).

• **Photon machines Analyte 193 Excimer Laser Ablation System** - The laser system is used for the ablation of solid material which is directly input to the Element XR high-resolution ICPMS.