ORNL – Expanding National R&D Capabilities

Sharon Robinson, PhD, P.E.

Oak Ridge National Laboratory

October 30, 2006

ORNL is DOE's largest multipurpose science and energy laboratory

- $1 billion budget
- 4,000 employees
- 3,000 research guests annually
- Nation's largest unclassified scientific computing facility

- Nation's largest science facility: the $1.4 billion Spallation Neutron Source
- Nation's largest concentration of open source materials research
- Nation's largest energy laboratory
- $300 million modernization in progress

ORNL is managed and operated by UT-Battelle

UT-BATTELLE
Limited Liability Company

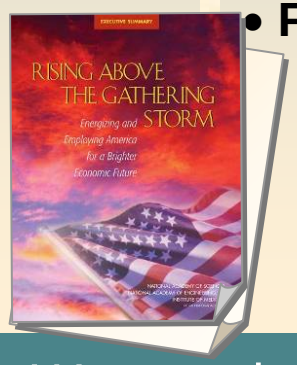
The University of Tennessee
Knoxville, Tennessee

Battelle
Columbus, Ohio

Presidential initiatives have formed DOE's and ORNL's mission priorities

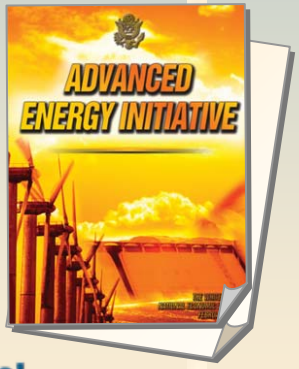
Science

- **Nanotechnology**
- **Materials sciences**
- **High-speed computation**
- **Biotechnology**
- **"Science to Energy"**



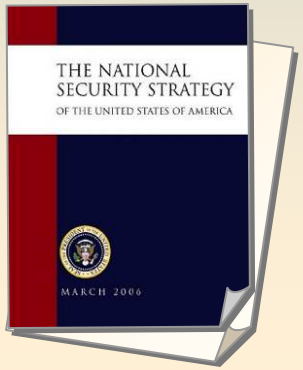
Energy

- **Nuclear**
  - **Support new reactor construction**
  - **Move spent fuel**
  - **Execute GNEP**
- **Clean coal**
- **Hydrogen**
- **Biomass**
- **Fusion**



National security

- **Nonproliferation and counterterrorism**
- **Weapons program: Complex 2030**



We are involved across the board

Responding to the President's call for bioenergy R&D

- **The Joint Institute for Biological Sciences is under construction**
  - **Vision for west campus development is taking shape**
- **We are preparing a proposal for a Genomics:GTL bioenergy center**

Expanding national security emphasis

- **Our capabilities in chemical and biological defense are in demand**
- **Significant and increasing support to the Department of Homeland Security**
  - **Protective Security Analysis Capability program**
  - **Southeast Regional Research Initiative**
- **The new Multiprogram Research Facility is nearing completion**

The Leadership Computing Facility is advancing to the petascale

- **Cray XT3 Jaguar upgrades are on schedule**
  - **Expansion to 54 TF complete**
  - **100 TF by November 2006**
  - **250 TF in 2007**
- **We have a role in 22 SciDAC-2 projects**
- **The 1-PF Cray Baker system will be deployed in 2008**
- **Other agencies have expressed interest in locating petascale machines at ORNL**

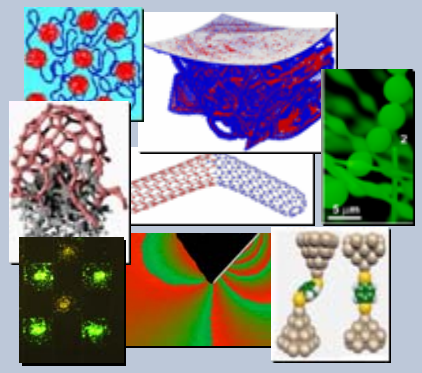
The research community is using the Leadership Computing Facility

Boeing **Engineering physics: Large-scale computational tools for flight vehicles**	Harvard **Life sciences: Molecular dynamics of molecular motors**
General Atomics **Fusion energy: Plasma turbulence**	Dreamworks Animation **Computer science: Ray tracing**

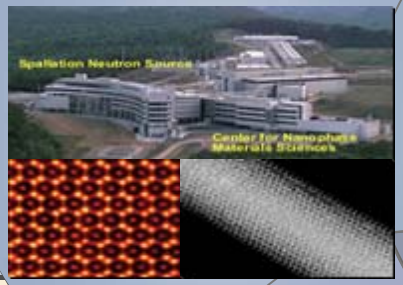
Nanotechnology: Integration from basic research to marketable products

Nanoscale Science

Synthesis, Modeling, Characterization and Design



Existing:
Basic Research



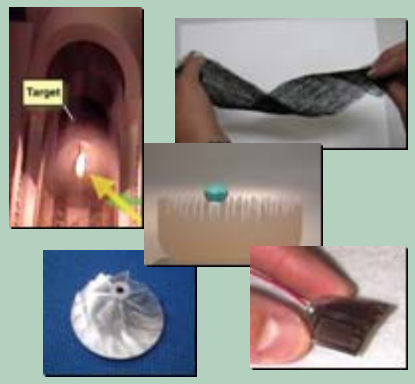
CNMS & SNS

Nanomanufacturing

Process development, Scale-up, Real-time characterization tools, Proof of concept & Prototypes

Proposed:
DOE Applications-Driven Nanomanufacturing R&D

Nanomanufacturing Technology Innovation Partnerships



Expected Outcomes

- **Energy Supply**
  - **Examples: Catalysts & Power Transmission – 2 quads/yr each**
- **National Competitiveness**
  - **Low-cost manufacturing**
- **Environmental Stewardship**

S&T Park

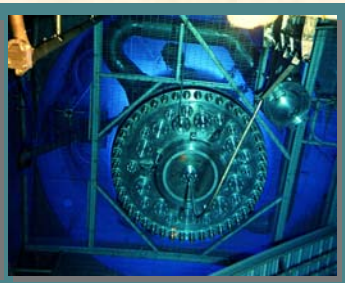
Emerging:
Industrial Commercial Development

Energy Applications

Electric Grid, Biofuels, Solar Power, Solid State Lighting, Energy Storage, Power Electronics, Transportation, and CO_2 Sequestration

$2B in new investment places ORNL at forefront of the nanotech revolution

DOE's first nanoscience center



World's foremost neutron science center

Leadership-class computing

- **New tools for atomic-scale characterization**
- **New capabilities for single atom/molecule manipulation**
- **Computational access to large systems of atoms and long time scales**
- **Convergence of scientific-disciplines at the nanoscale**

Creating a set of scientific synergies that will accelerate the process of discovery thus providing a unique opportunity to understand nanoscale materials, assemblies, and phenomena

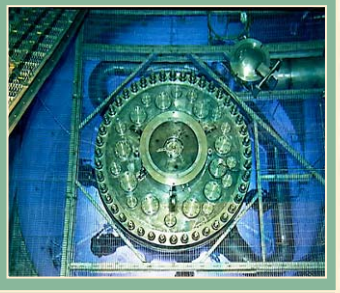
We are developing and deploying world-class tools for nanoscale R&D

Spallation Neutron Source

- High-intensity neutrons for materials research at the nanoscale
- 1.4 MW of beam power on target
- 16 instruments

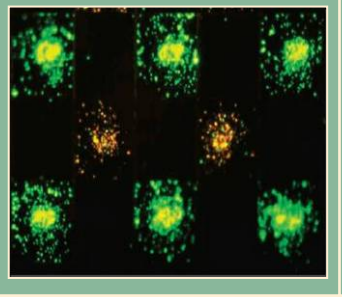
High Flux Isotope Reactor

- The nation's leading research reactor
- World-class for neutron scattering



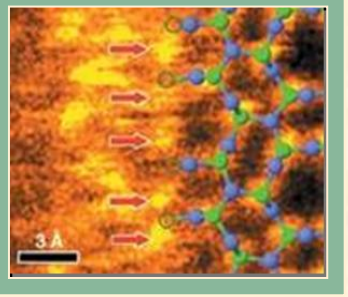
Center for Nanophase Materials Sciences

- $65M facility begins operations in October 2005
- 75 user projects already under way



Ultrahigh-resolution microscopy

- Advanced Microscopy Laboratory
- Aberration-corrected electron microscope
- World-record resolution: 0.6 Å

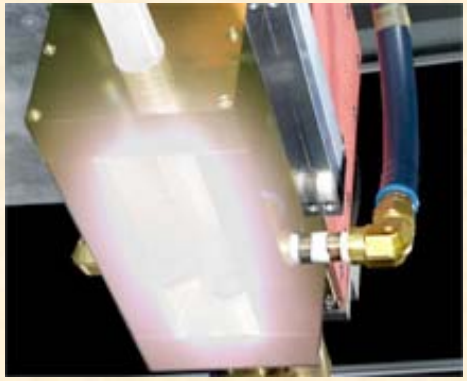


Nanoscale Science & Technology Laboratory Clean Room Facility

- **Houses full range of processes and fabrication techniques**
  - **Lithography and etching**
  - **Thin-film deposition**
  - **Compound semiconductor-based device fabrication**
  - **Scanning Probe Microscopy, AFM, and other microscopic evaluation techniques**
- **Supports a wide range variety of thin-film, solid state electronic, and genome research**

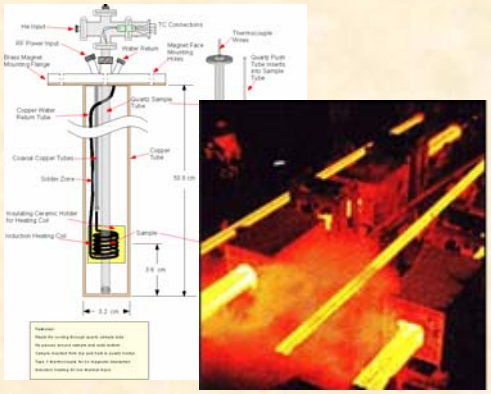
ORNL Advanced Materials Processing

Goal: Enable U. S. expansion of energy efficient advanced materials and processing/manufacturing by focusing on advanced breakthrough processing technologies



Functionalizing NanoMaterials

Surfacing & Interference Metallurgy



Magnetic Field Processing for Alloys

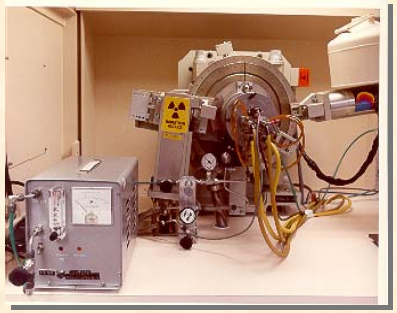
Laser Assisted Friction Stir Welding

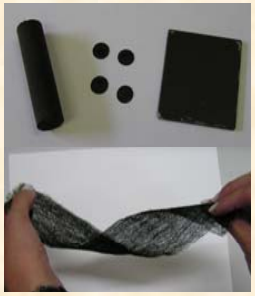
Electron Beam Processing
Nonthermal Processing of Composites

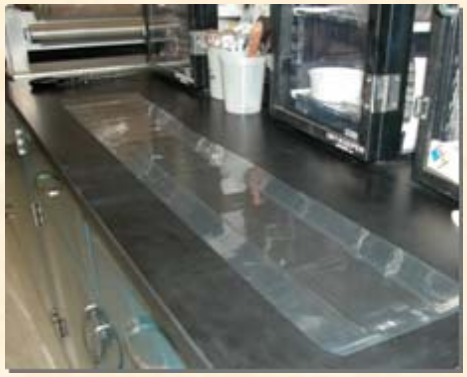
Twin Roll Casting of Advanced Alloys

Chemical processing for nanomaterials engineering

- **Laser-assisted processing**
- **Field-directed processing (Electrical, Magnetic, Microwave…)**
- **Thermal processing**
- **Electrochemical processing**
- **Molecular assembly-assisted processing**

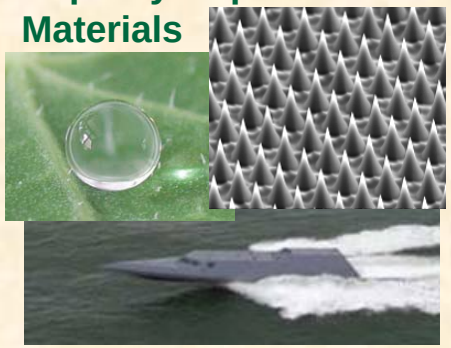




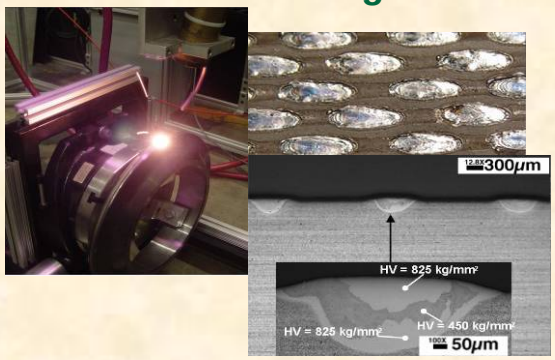


ORNL is moving nanotechnologies closer to the marketplace

Superhydrophobic Materials



Wear Resistant Coatings



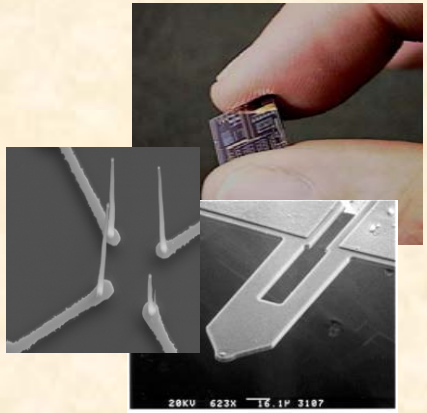
Solid State Lighting

Nanofermentation

Prosthetics

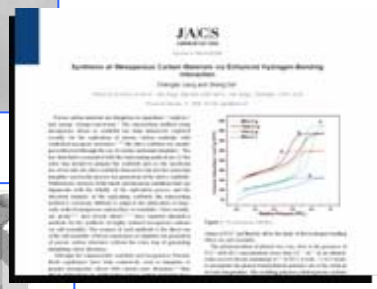
Energy Production, Storage, & Conversion

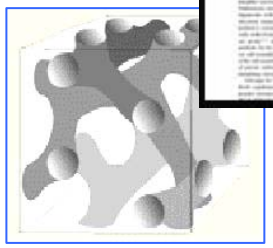
Sensors & Diagnostics



Nanomaterials to Ultracapacitors

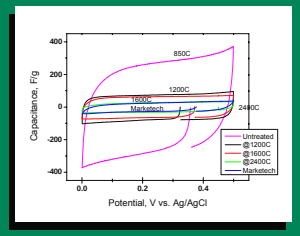
Basic Research

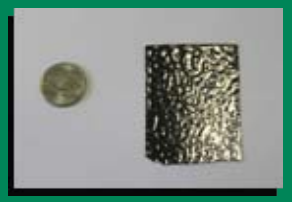




Nanoscale Science Discovery

Applied R&D





Nanomanufacturing

Maturation & Deployment

Implementation of Energy Nanotechnologies

Ionic Liquids as Extractants for Chemical and Radiochemical Separations & Detection

ORNL reports convenient / efficient synthesis route

Cs Extraction Results* using BoBcalixC6 in Ionic Liquid Solvents

Concentration of BoBcalixC6 in $BuMeIm^+Tf_2N^-$	Initial aqueous phase composition	D_{K^+}	D_{Cs^+}	D_{Na^+} or $D_{Sr^{+2}}$	D_{Cs^+}/D_{K^+}
7.7 x 10^{-3} *M*	150 ppm K^+, Cs^+, and Na^+	3.7	162	0	44
7.7 x 10^{-3} *M*	150 ppm K^+ and Cs^+	2.8	118	-	43
7.7 x 10^{-3} *M*	150 ppm K^+, Cs^+, and Sr^{+2}	3.0	102	0	35

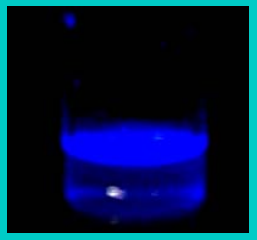
BoBcalixC6 Concentration	D_{Cs^+} *R* in $RMeIm^+Tf_2N^-$				chloroform
	Propyl	Butyl	Hexyl	Octyl	
1.3 x 10^{-2} *M*	140	130	57	18	0.034

*The distribution coefficient, D_M, is defined as $D_M = \frac{[Concentration\ of\ M\ in\ carrier\ solution]}{[Concentration\ of\ M\ in\ aqueous\ solution]}$.

Extractant is >4000 times more effective in ionic liquid than in conventional solvent

Preliminary testing indicates viability of SX in centrifugal contactors with ionic liquids

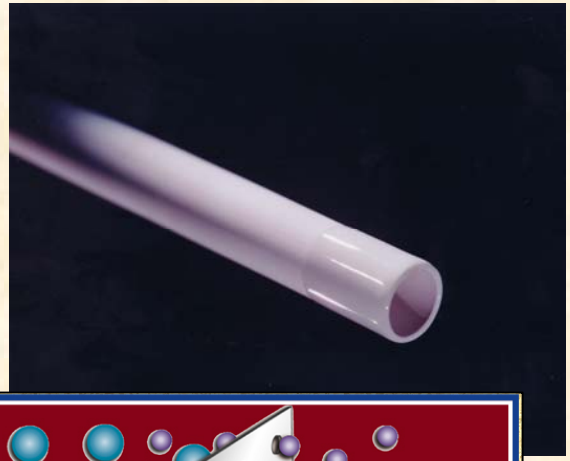
Nonflammable, nonvolatile ionic liquids can be used as the basis of solvents for efficient extraction and concentration of actinides and fission products.

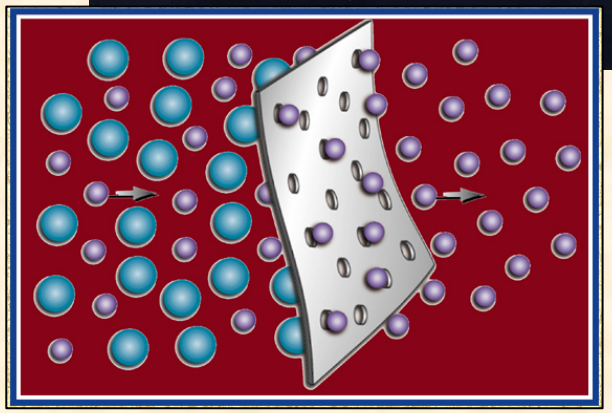


Scintillating ionic liquid allows preconcentration and detection of actinides and fission products

Membranes: Low-energy Separations

- Materials engineered at the molecular scale allow selective, energy-efficient separations at high throughput
- Further advancement and application will be achieved through
  - Improved understanding of transport mechanisms at the nanoscale
  - Advances in nanomanufacturing and processing to fabricate media with desired functionality
- **Potential Opportunities and Energy Savings:**
  - Replacing high-energy-usage separation methods by less energy-intensive methods – membranes, extraction, or adsorption – could result in substantial future energy savings.
    - Petroleum & chemical industry distillation : 1 Quad
    - Black liquor concentration: 0.11 Quads
  - Other opportunities:
    - Hydrogen recovery from mixed gas streams, thermochemical cycles, desalination, solid oxide fuel cells



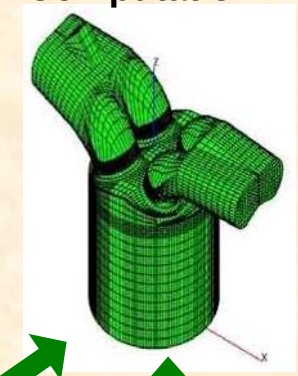


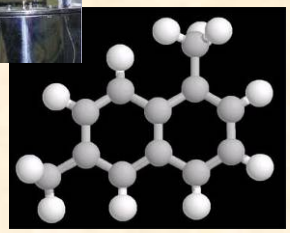
Molecular sieve membrane for separating gas molecules

Alternative Fuels & Feedstocks:

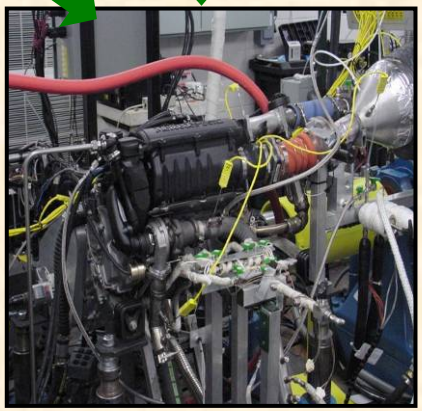
Coupling fuel chemistry, computations, and experiments to develop new fuels and chemical feedstocks

Computation





Fuel Chemistry

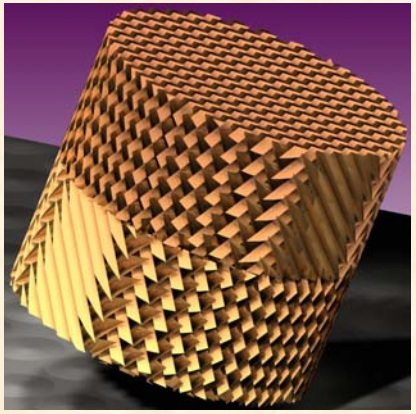


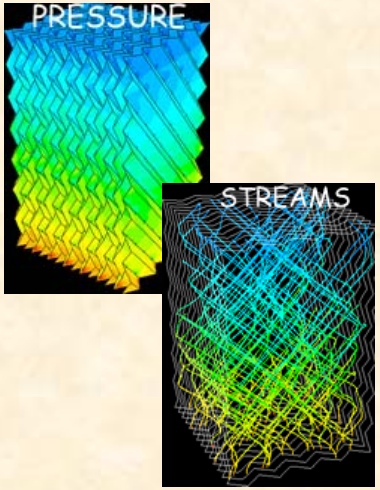
Experimental

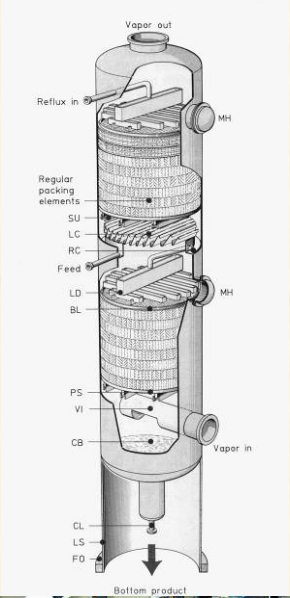
- **Establish capability to enable the use of non-petroleum based alternative fuel formulations for advanced combustion regime engines**

- **Effort combines capabilities in fuel chemistry and engineering computations with established strength in experimental IC engine R&D to create a unique capability for ORNL**

U.S. DISTILLATION INDUSTRY OF THE FUTURE



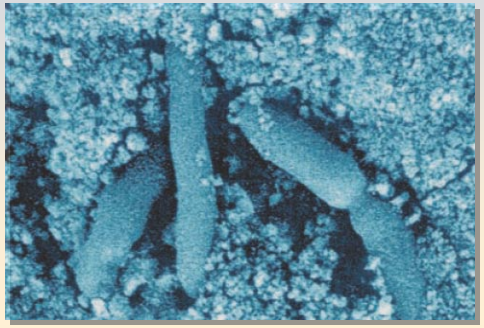
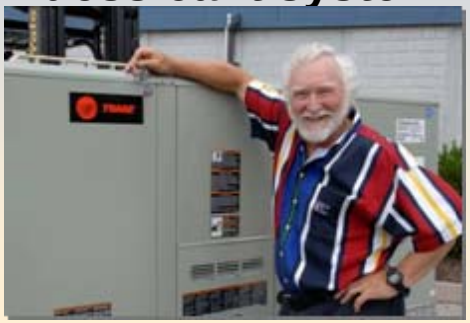




- Energy saving through modern computer-aided design
- Automated high-fidelity complex geometry modeling of industrial packing
- Large scale 3-D two-phase counterflow simulation and experimental validation
- Industrial scientific computing via dedicated cluster paradigm
- Licensed GraSPI to Fluent

Office of Industrial Technologies of the US Department of Energy

Six ORNL innovations received R&D 100 awards for 2006

Hybrid solar lighting 	**LandScan Global Population Database** 	**Metal Infusion Surface Treatment**
NanoFermentation: **Bacterial production of nanocrystalline powders** 	**TMA 6301, TMA 4701:** **Heat-resistant cast austenitic stainless steels** 	**Trane CDQ (Cool, Dry, Quiet) dessicant system** 

Discussion