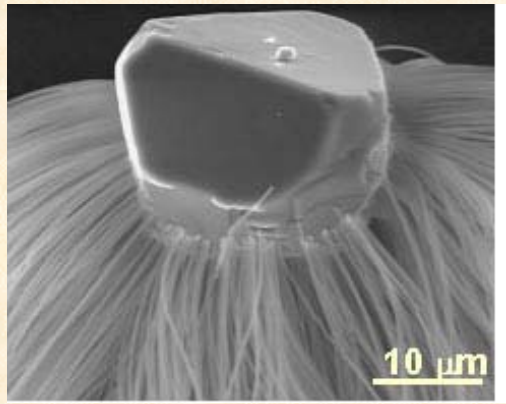
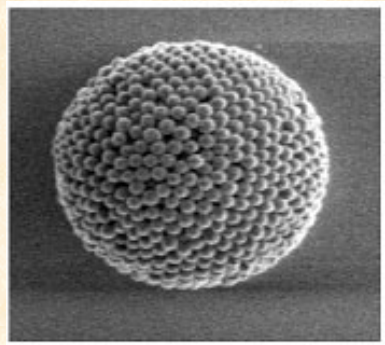
Chemical Sciences at ORNL

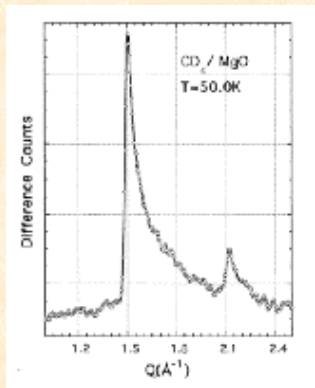
(Largest BES funded program in the National Laboratory System)



- **World class capabilities**
  - -Mass spectroscopy
  - -High pressure and temperature chemistry
  - -Solution chemical synthesis of materials
  - -Meso-structured high surface area materials
  - -Catalysis



- **Synthesis**
  - -Boron and silicon hydrides, borazines, borane amines, silyl amines
  - -Polymers and organic/inorganic hybrid materials
  - -Nanostructured materials



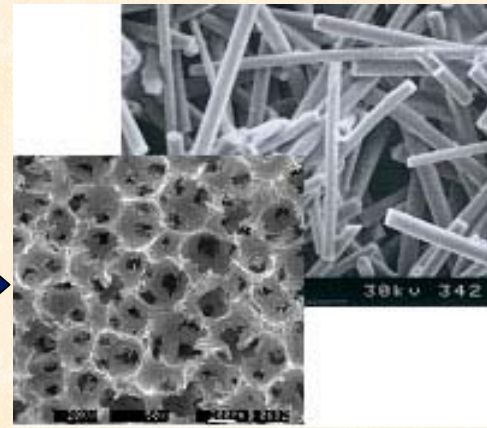
- **Characterization**
  - -Solid-state NMR of carbon materials
  - -Structure and dynamics of small molecules on nanostructured materials in vacuum and solution using neutron scattering
  - -Adsorption isotherms

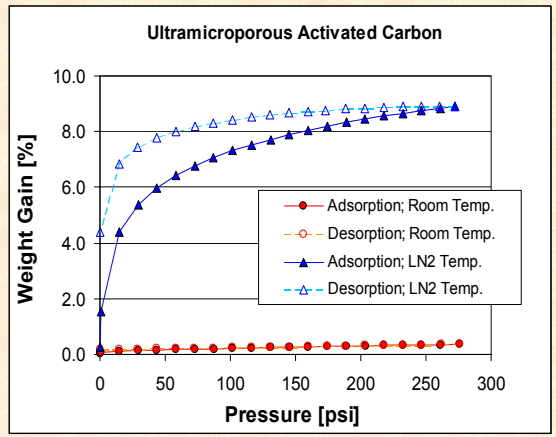
UT-BATTELLE

Carbon Materials Research Group at ORNL Largest in the United States

Carbon Group Capabilities:

- **Novel synthesis of carbons**
  - Nano-structured carbon
  - Templated microporous carbon
  - Foams
  - Graphites
  - Fibers
- **Performs advanced carbon characterization**
  - HRTEM
  - SAXS/SANS
  - XRD
- **Adsorption and separation apparatus**
  - Autosorb-1C (Volumetric)
  - IGA (Gravimetric): LN_2-1000°C; up to 300 psi (on-line mass spec)
  - High pressure volumetric system, up to 3000 psi





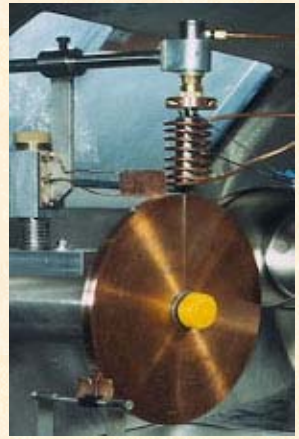
HYDROGEN ADSORPTION ON MICROPOROUS CARBON

Alloy Design and Development at ORNL

Alloy Development and Processing Capabilities

- Fabrication capabilities
  - Arc-casting, melt spinning, inert gas condensation microalloying
  - High-energy ball milling with environmental control
  - High-density infrared processing of alloys
  - Laser-processing for metastable materials
  - Experience with difficult-to-process hydrogen storage materials, such as $MgNdNi_4$
- Combinatorial chemistry/Molecular Engineering of Metal hydrides
  - PLD, CVD
  - XPS
  - IR imaging
- Modeling of Complex Phenomena
  - Thermodynamic, and kinetic modeling combined with artificial intelligence techniques for alloy design
  - Describe the relation between composition, structure, and properties
  - Describe complex, multi-length and time scale processes

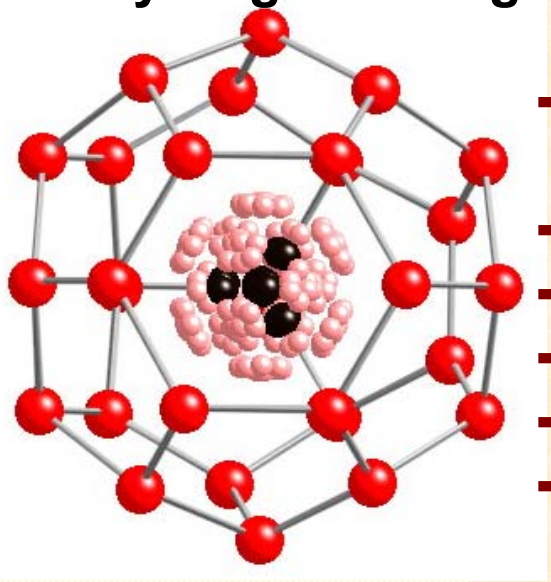
Set-up for melt-spinning of LiH. **ORNL/Y-12 Largest LiH Production Facility in US**



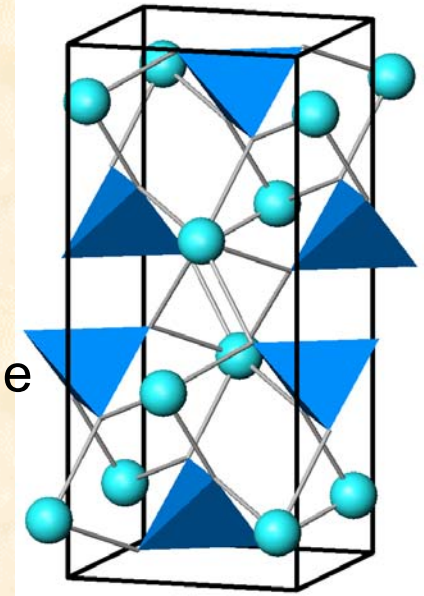
Attritor Mill For Powder-Processing

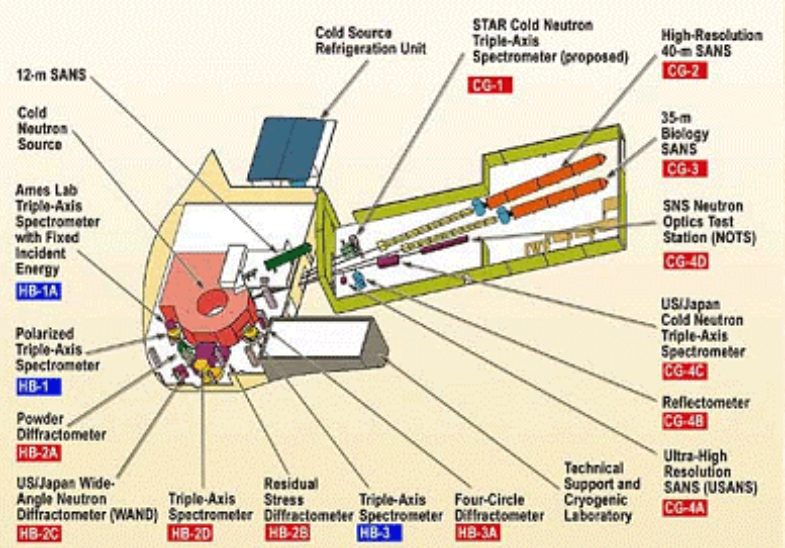
Neutron Scattering at Oak Ridge National Laboratory

Characterize hydrogen storage materials by in-situ neutron scattering studies.



- quantitative phase analysis
- phase transformations
- thermal expansion
- hydrogen positions
- vibrational modes
- large & complex sample environments





Neutrons are highly penetrating and "see" hydrogen better than x-rays

A U.S. Department of Energy multilaboratory project

Spallation Neutron Source

The next-generation neutron-scattering facility for the United States

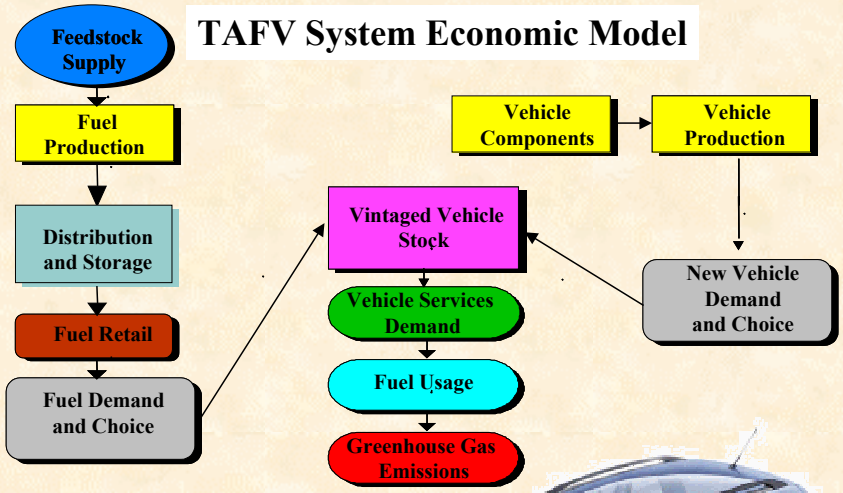
SNS

UT-BATTELLE

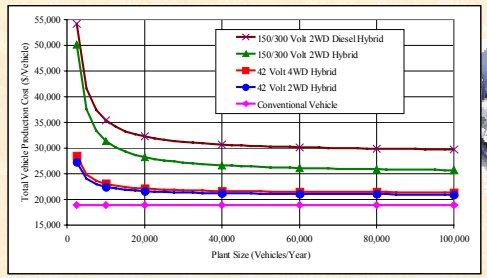
Upgraded High Flux Isotope Reactor (HFIR)

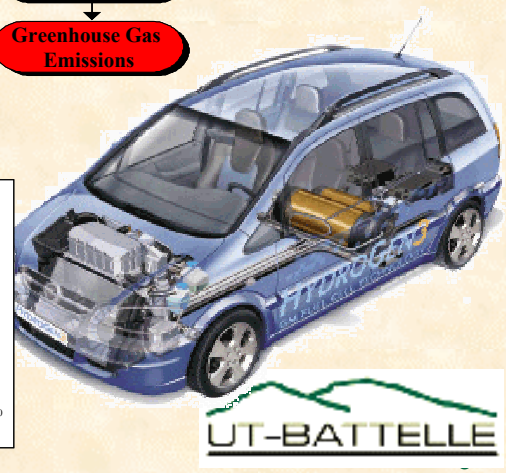
ORNL Has Extensive Economics Experience and Capability

- **System Costs**
  - Engineering cost analysis
  - Materials supply and economics
  - Learning and economies of scale
- **Cradle-to-Grave Effects**
  - Supply chains, Logistics and transportation
  - Recycling economics
  - Life-cycle assessment
- **Market Prospects and Acceptance**
  - Consumer choice and acceptability
  - Market modeling and assessment, supply and demand balances
  - Technology choice and transitions
- **R&D Benefits assessment**



Component and Vehicle Scale Economies: Cost vs. Plant Size





UT-BATTELLE