EXECUTIVE SUMMARY

- Preview of Poster Session
- Introduction to CMT
- Map of Building 205

Poster Session
for
Materials Science Division

April 26, 2004
2:00 p.m. to 4:00 p.m.
Building 205

Hosted by
Chemical Engineering Division
David Lewis, Director

PREVIEW

Catalysis Research
Point of Contact: Chris Marshall (2-4310)

The Chemical Engineering Division has unique capabilities for studying heterogeneous catalytic systems under operating conditions (in-situ) to understand the reaction mechanisms and to lead to improvements in both activity and selectivity. These capabilities include several high-pressure reactor cells for both plug flow and membrane reactors, diffuse reflectance IR (DRIFTS), temperature-programmed reactors, and a combinatorial reactor system. Extensive use of in-situ capabilities at the MR-CAT at the Advanced Photon Source compliment in-house characterization abilities. Expertise is needed to understand the nature of the metallic material used under working catalyst conditions and the nature of the metal-support interaction that controls many of the catalyst properties.

Tour of Laboratory B-101
Featured Posters

- Catalytic Destruction of Chemical Threats in Human-Occupied Spaces
- New Supports for the Catalytic Removal of Sulfur from Heavy Oils
- Bifunctional Catalysts for the Selective Catalytic Reduction of NO by Hydrocarbons

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Hydrogen
Point of Contact: Debbie Myers (2-4261)

Our programs in support of the hydrogen initiative cover production, purification, and storage. Thermochemical cycles are being investigated for stationary hydrogen production. The most promising candidate has proved to be a family of three hybrid cycles based on copper and chlorine chemistry operating at ~550°C. The reforming of gasoline, natural gas, and other conventional or alternative fuels via catalytic processes is being investigated for stationary and on-board hydrogen production for residential and vehicular fuel cell power systems. Research in hydrocarbon fuel processing for fuel cells also includes hydrogen purification via water-gas shift catalysis. Current projects in hydrogen storage focus on the development of nanoparticulate aluminum and aluminum-containing compounds with structures that can maintain the size of the alane hydride phase within the nanometer regime. The Division's capabilities in the hydrogen area include expertise in process, catalyst, and materials development and characterization.

Tour of Laboratory A-101
Featured Posters

- Production of Hydrogen from Water with Low-Temperature Thermochemical Cycles
- Fuel Processing Catalyst Development
- Oxidation States of Pt in Ceria-Supported Pt Water-Gas Shift Catalysts
- Lightweight and Robust Hydrogen Storage Materials for Automotive Fuel Cells

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Nano-Materials
Point of Contact: Michael Kaminski (2-4777)

We are working with several Divisions at Argonne and outside institutions to develop magnetic nanospheres that can be safely injected into the human vasculature. These magnetic nanospheres are smaller than red blood cells and can carry selective surface receptors for targeting cells such as binding to circulating cancer cells, blood-borne biological toxins, or internalized radioactivity. Because of their magnetic moment, the nanospheres can be removed from circulation by a simple extracorporeal magnetic filter, thus providing a concentrated analyte for early detection or providing treatment to the patient. In another application, the nanospheres can carry a drug payload into the vasculature. By positioning magnets external to the body, the nanospheres can be concentrated in the region of disease to increase the efficacy of the drug and decrease common side-effects. Combining physical magnetic positioning of the drug-loaded nanospheres with biological receptors such as monoclonal antibodies, a synergistic effect may be realized to improve treatment outcome.

Featured Posters, C-Wing

- Using Nanoscale Technology to Help Stroke Victims: Prototype Nanoparticles for Future Magnetically Guided, Targeted Tissue Plasminogen Activator Stroke Therapy
- Searching for Improved Treatment Options for Human Internal Decontaminations: A Nanoscale Approach

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High Temperature Materials
Point of Contact: Jude Runge (2-3430)

Innovative materials solutions for demanding high temperature and corrosive environments will be needed for the technologies being developed in the Generation IV and the Advanced Fuel Cycle Initiative Programs. Various ceramic and cermet materials have been investigated and tested in the development of an inert anode for electrolytic reduction of spent fuel. A new process to manufacture uranium trichloride (UCl_3), necessary for electrorefiner operation, has also been developed. Various structural materials are being investigated and tested in flowing molten lead and lead alloys, as well as in molten salt, at temperatures up to 800^{o}C. Coatings and coating methods are also being researched for substrates that exhibit thermomechanical stability that may not be corrosion-resistant. The ramifications of successful development of high- temperature materials are far-reaching, as all of the new reactor concepts require corrosion-resistant, thermally stable materials.

Featured Posters, A-Wing

- Anode Development for Electrolytic Reduction of Spent Oxide Fuel
- Performance of Structural Materials to Enable the Electrolytic Reduction of Spent Oxide Nuclear Fuel in a Molten Salt Electrolyte
- Performance of Structural Materials in Lead-Based Reactor Coolants at Temperatures up to 800^{o}C Chemical Vapor Deposition of Niobium Coating on Microspheres
- Large-Scale Production of UCl_3 for Use in Pyroprocessing Spent Nuclear Fuels

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Electrochemical Materials Research
Point of Contact: Chris Johnson (2-4787)

Advanced batteries and fuel cells are key enabling technologies for fulfilling our nation's future energy conversion and storage needs. Batteries and fuel cell materials deliver power from an external current produced by an internal electrochemical reaction. The research and development of electrochemical materials properties are critically important for new discoveries and progress in these areas. The Battery and Fuel Cell Technology sections in the Chemical Engineering Division encompass a broad multi-disciplinary group of scientists and engineers that are focused on electrochemical technologies. Our world-class facilities, capabilities and technical skill encompass activities as diverse as conducting basic structural research on battery electrodes at the Advanced Photon Source (APS), to the electrochemical engineering and testing of battery packs for hybrid electric vehicles, to the development of improved solid oxide fuel cell materials for auxiliary power units for trucks. The overlap and integration of electrochemistry with materials science summarizes the research in this session.

Featured Posters, A-Wing

- Non-Precious Metal Electrocatalysts for Polymer Electrolyte Fuel Cells
- Dopant-Induced Stabilization of Rhombohedral $LiMnO_2$ against Jahn-Teller Distortion
- High Temperature Polymer Electrolyte Membranes
- Electron Transfer at the Border Between Intermetallic and Zintl Phases
- Metallic Bi-polar Plate-Supported Solid Oxide Fuel Cell (TuffCell)
- Coated Lithium Battery Materials: Towards Improvement in Interfacial Electrochemistry
- Measurement of Unknown Optical Rotatory Properties of CB Agents and Simulants Using Optical Polarimetry
- Miniature Rechargeable Battery for Bion® Microstimulator
- High-Voltage $Li[(Ni_{0.5-x}Co_x)Mn_{1.5}]O_4$ ($0 \le x \le 0.5$) Spinel Oxide Cathodes for Lithium Batteries

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Nuclear Magnetic Resonance
Point of Contact: Jerry Rathke (2-4549)

The Chemical Engineering Division has unique capabilities for in-situ, high pressure nuclear magnetic resonance spectroscopy and imaging. These capabilities have been used to explore catalysis mechanisms, novel reaction media formed by dispersing micelles in supercritical fluids, ion concentration gradients in electrochemical systems, and kinetic and thermochemical processes associated with hydrogen storage. These capabilities allow increased understanding at the molecular level of organometallic reaction mechanisms that can lead to improvements in industrial homogeneous and heterogeneous catalysts, batteries, and fuel cells. The solution-phase spectroscopic capabilities of the NMR Facility in CMT neatly complement the surface-science techniques available at the Argonne User Facilities (APS, IPNS, CNM, etc.) in the exploration of nanoscience at the earliest stage of self-assembly, and beyond.

Tour of Laboratories J-101 and J-102
Featured Posters

- Catalytic Olefin Hydroformylation in Supercritical Carbon Dioxide
- Gas Phase Micelles as Minireactors for Catalysis
- Investigations of Electrochemical Systems Using Novel Detectors: Toroid Cavity NMR Imagers

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Synchrotron Radiation and MR-CAT
Point of Contact: Jeremy Kropf (2-9398)

Experiments conducted at the APS Materials Research Collaborative Access Team (MR-CAT) support a broad array of the Division's programs. A particular emphasis has been placed on investigating functional material embodiments under relevant operating conditions such as batteries in charge or discharge mode, catalysts under actual reaction conditions, non-destructive analysis of partially and fully manufactured composite superconductors, and replications of radioactive material waste forms. As a consequence of the Division's decade-long involvement in the MR-CAT, specialized capabilities (designed to meet our specific needs) have been developed that facilitate the measurement of x-ray absorption spectra and x-ray scattering in-situ as a function of temperature, pressure, and chemical environment. Examples of these capabilities will be presented in this topical group. We expect the MR-CAT at the APS to remain a critical resource for our research and development activities in areas that pertain to the hydrogen economy, Generation-IV nuclear reactor technology, nanotechnology, fuel cell systems, and catalysis for chemical and environmental applications.

Featured Posters, J-Wing

- Non-Destructive Transmission X-Ray Diffraction Analysis of the Silver-Sheathed Bi-2223 Composite Superconductor
- The Nature of Molten Chloride Salt Occlusion by Zeolite 4A
- Metal Oxide Electrode Multi-Electron Transfer Process
- In Situ X-Ray Absorption Spectroscopy of Electrochemically Induced Phase Changes in Lithium-Doped InSb
- In Situ XAFS Analysis of the Temperature-Programmed Reduction of Cu-ZSM-5
- A Bent Silicon Crystal in the Laue Geometry to Resolve X-Ray Fluorescense for X-Ray Absorption Spectroscopy
- Using Raman Spectroscopy and X-Ray Diffraction Space Mapping to Explore Epitaxy, Strain, and Twinning in $MBa_2Cu_3O_{7-x}$ Coated Conductor Embodiments
- In Situ Real-Time XAFS Characterization of Noble Metal Catalyst Impregnation

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Nuclear Materials Characterization

Point of Contact: Jeff Fortner (2-5594)
For TEM: Nancy Dietz (2-9798)

Through years of research into the corrosion mechanisms of commercial spent nuclear fuel (CSNF) and waste forms, we have developed unparalleled tools and techniques for the characterization of radioactive materials. Applications of transmission electron microscopy and the novel “bent-Laue analyzer” detection scheme developed in collaboration with the Illinois Institute of Technology at the MR-CAT will be highlighted. The brightness of the APS facility in the high-energy x-ray regimes makes it ideal for investigating radionuclide systems, which have relatively high-energy absorption edges, and which must be carefully encapsulated for radiological safety. These data, for the first time, have allowed direct observation of oxidation state, coordination environment, and site symmetry of fission product and actinide elements in CSNF. We anticipate these characterization tools will continue to support our repository relevant research and play an important role in meeting the nuclear materials research needs of advanced reactor systems.

Featured Posters, J-Wing

- Trace Element Chemistry in Spent Nuclear Fuel Using X-ray Absorption Spectroscopy
- Neptunium Substitution into the Structure of Alpha-U_3O_8
- Transmission Electron Microscopy in the Chemical Engineering Division

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The Chemical Engineering Division
at Argonne National Laboratory

The Chemical Engineering Division is one of six divisions within the Engineering Research Directorate at Argonne National Laboratory, one of the U.S. government's oldest and largest research laboratories. The University of Chicago oversees the laboratory on behalf of the U.S. Department of Energy (DOE). Argonne's mission is to conduct basic scientific research, to operate national scientific facilities, to enhance the nation's energy resources, to promote national security, and to develop better ways to manage environmental problems. Argonne has the further responsibility of strengthening the nation's technology base by developing innovative technology and transferring it to industry.

The Division is a diverse early-stage engineering organization, specializing in the treatment of spent nuclear fuel, development of advanced electrochemical power sources, and management of both high- and low-level nuclear wastes. Additionally, the Division operates the Analytical Chemistry Laboratory, which provides a broad range of analytical services to Argonne and other organizations.

The Division is multidisciplinary. Its people have formal training in chemistry; physics; materials science; and electrical, mechanical, chemical, and nuclear engineeing. They are specialists in electrochemistry, ceramics, metallurgy, catalysis, materials characterization, nuclear magnetic resonance, repository science, and the nuclear fuel cycle. Our staff have experience working in and collaborating with university, industry and government research and development laboratories throughout the world.

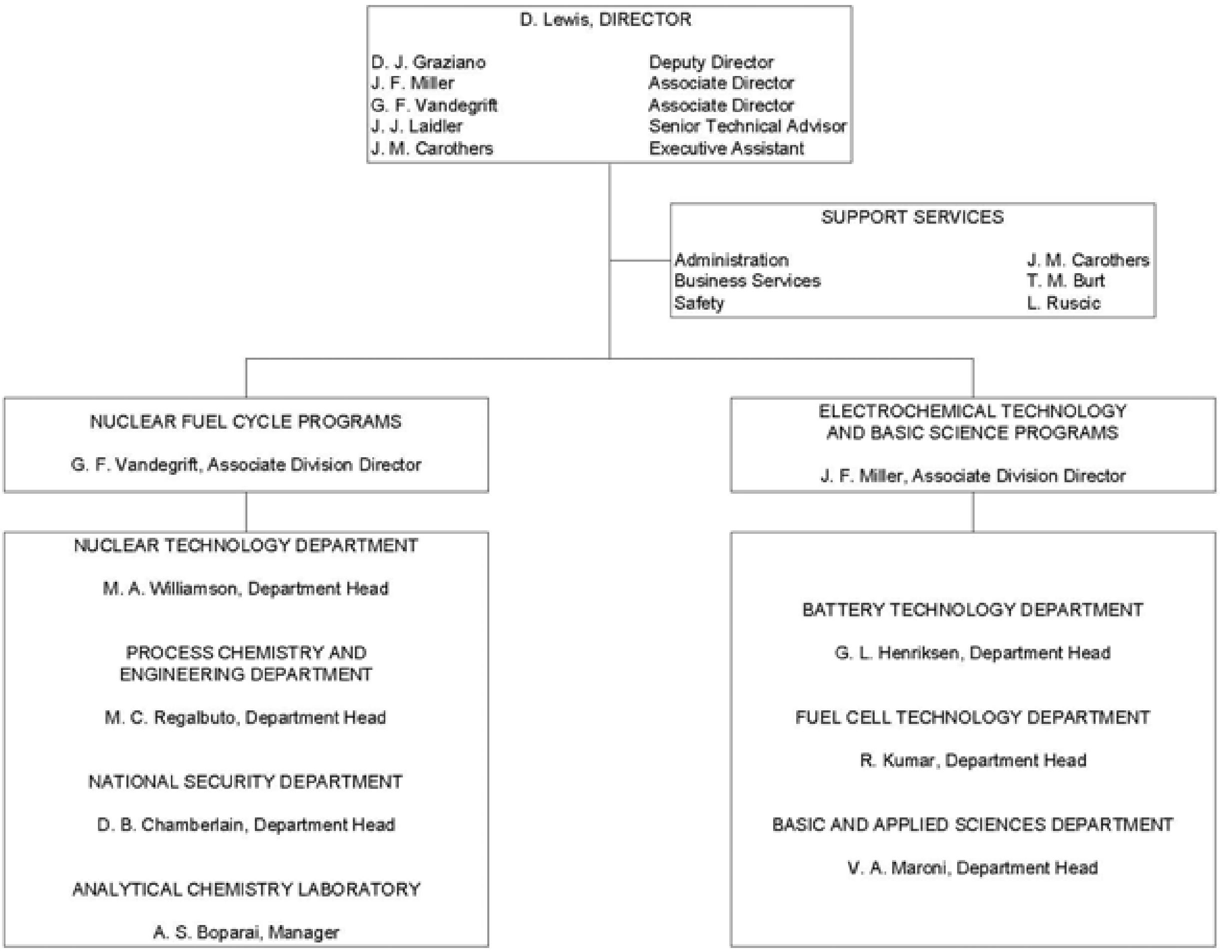
Our wide-ranging expertise finds ready application in solving energy, national security, and environmental problems. Division personnel are frequently called on by governmental and industrial organizations for advice and contributions to problem solving in areas that intersect present and past Division programs and activities.

Currently, we are engaged in the development of several technologies of national importance. Included among them are:

- Advanced lithium-ion and lithium-polymer batteries for transportation and other applications,
- Fuel cells, including the use of an oxidative reformer with gasoline as the fuel supply,
- Production and storage technologies critical to the hydrogen economy,
- Stable nuclear waste forms suitable for storage in a geological repository,
- Threat attribution and training relative to radioactive dispersal devices ("dirty bombs"), and
- Aqueous and pyrochemical processes for the disposition of spent nuclear fuel.

Other important programs are focused in superconductivity, catalysis, nanotechnology, and nuclear materials.

During fiscal year 2003, CMT had an annual operating budget of approximately $36 million. Of that, more than 90% was from DOE and the remainder from other government agencies and private industry.



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Welcome to the Chemical Engineering Division!