ChemMatCARS

ChemMatCARS:
A Synchrotron Resource for Chemistry and Materials Research at the Advanced Photon Source
NSF/DOE CHE-0535644

P. J. Viccaro, PI

NSF Light Source Facilities Panel

January 9-10, 2008

Outline

- Scope of facility
- Mission/funding
- Communities served
- Challenges

http://cars.uchicago.edu

AUSTRALIAN SYNCHROTRON RESEARCH PROGRAM

Advanced Photon Source at Argonne National Laboratory

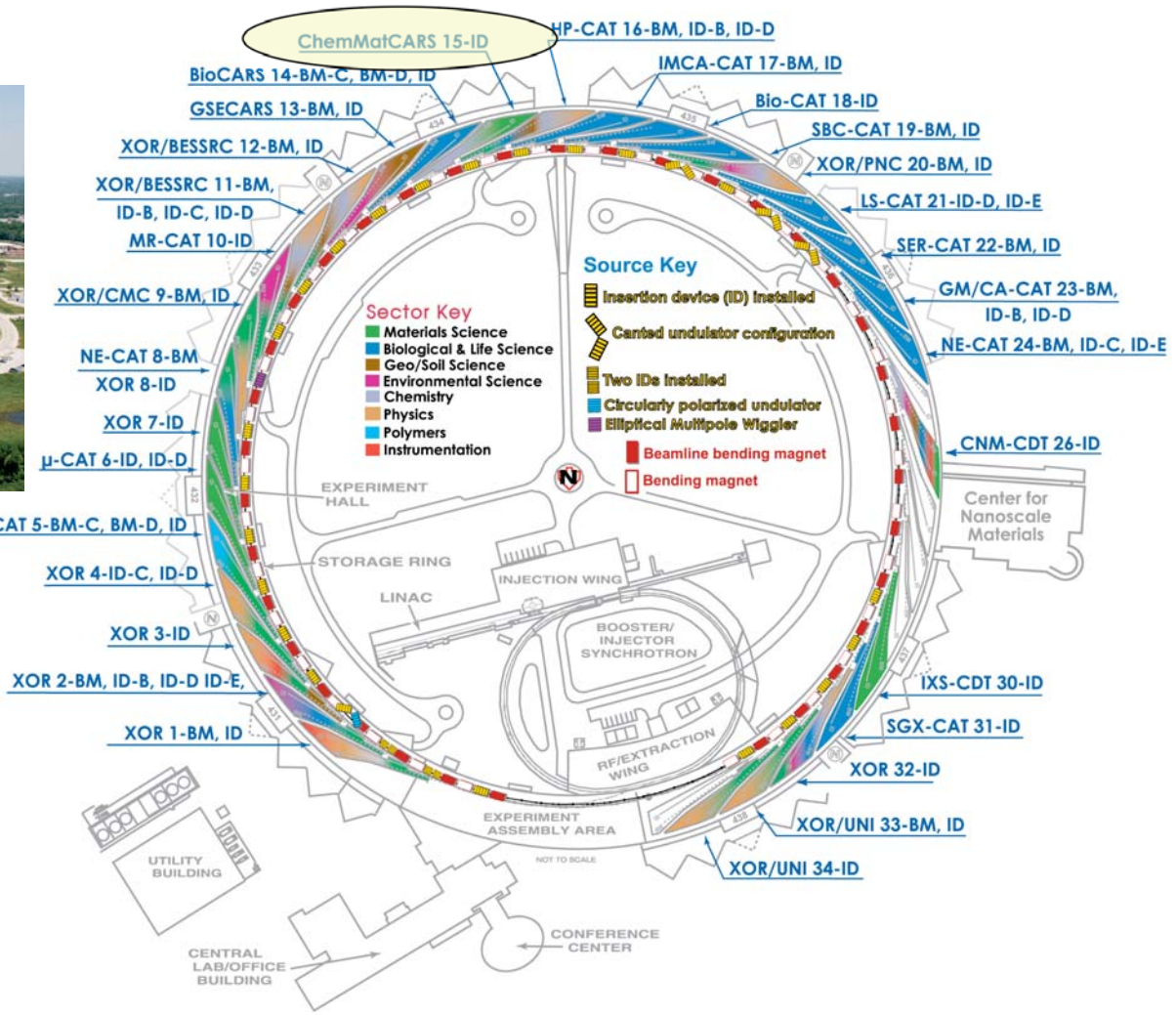
ChemMatCARS: Part of the University of Chicago
Center for Advanced Radiation Sources
APS Sectors 13, 14, 15, 17

GSECARS (13)
Geophysical and Environmental Science

BIOCARS (14)
Macromolecular Crystallography

CHEMMATCARS (15)
Chemistry and Material Science

IMCA-CAT (17)
Pharmaceutical Consortium



ChemMatCARS: One of many sectors

ChemMatCARS

- Operates and is funded as **NSF/DOE National User Facility** with targeted scientific communities
- It is a multi-technique facility developed in collaboration with the targeted communities
- All beamtime allocation is based on the Advanced Photon Source General User Proposal Review system. There are no "owner-users".
- Facility is open to scientists from the US and abroad

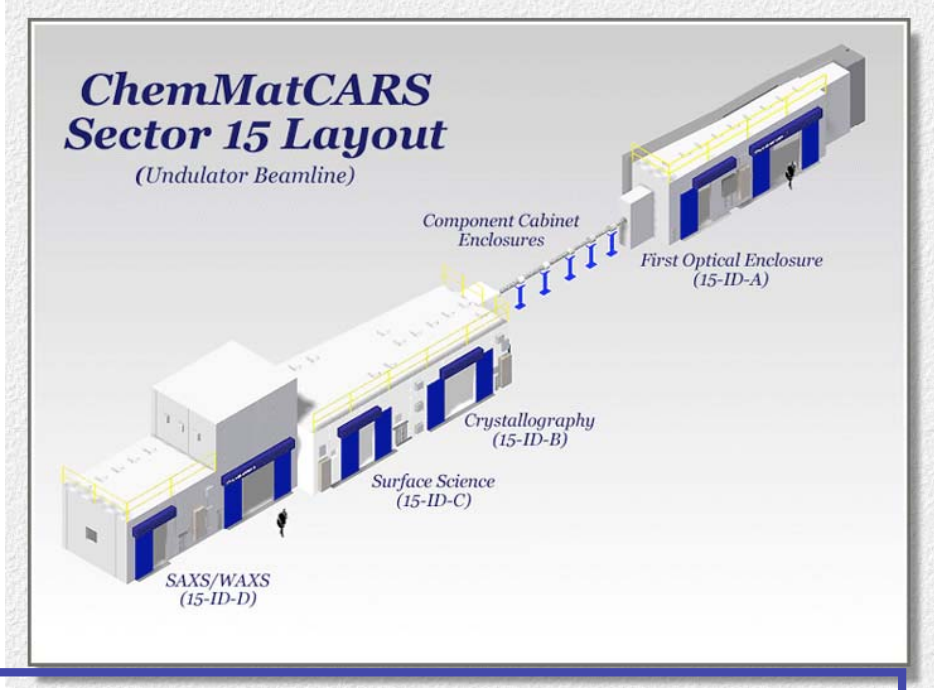
Mission Guidelines

- Experimental facilities must align with community scientific thrusts
- Training, Dissemination and Outreach
  - Development of the community
  - Workshops, Schools, etc.
- Interns residing at the facility
- Training of graduate students
- Outreach to underrepresented groups

Additional partnerships formed by the facility are governed by the NSF/DOE National User Facility Mission Guidelines

Only undulator port developed

- **Three experimental stations**
- **Tandem arrangement with one station accepting beam at a given time**
- **1 shift switchover between techniques**



Techniques available through APS General User program

- **Chemical crystallography-single crystal diffraction**
  - Chemical (micro) crystallography in 15-ID-C (turn-key) in collaboration with V. Young (U. of Minnesota), M. Pink (U. of Indiana), P. Turner (U. of Sydney)
  - Charge density capability in collaboration U. of Åarhus, Denmark
  - Time-resolved photo chemistry (P. Coppens, SUNY Buffalo)
- **Surface scattering /15-ID-C**
  - Wide q-range reflectivity and in plane scattering
- **Small angle x-ray scattering and wide angle x-ray scattering /15-ID-D**
  - Flexible, low noise, large q-range
- **New time-resolved thrust: Light Modulated XAFS (Jim Penner-Hahn, U of Mich.)**

Major Funding Sources

- 1996-2009: NSF (Chemistry and DMR)/DOE (BES-Materials) for partial funding of the construction of undulator beamline and infrastructure **(CHE-9522232)** and for operations (**CHE 0087817** and **CHE 0535644)**, CoPIs included: S. A. Rice, P. Perhsan, B. Chu, P. Coppens, T. Russell, M. Schlossman
- 1996-2009: Australian Synchrotron Research Program (ASRP) one-time capital ($1M) and operational support ($150K/year and seconded scientist at ChemMatCARS through 2009). This partnership resulted in creation of a SAXS-based synchrotron community in Australia which is currently developing a beamline at the Australia Synchrotron Source
- 1996: NSF ARIP grant jointly to BioCARS and ChemMatCARS for Crystallographic Data Acquisition Instrumentation development
- 1998: NSF MRI grant to Northern Illinois Univ. (S. Mini, PI) and ChemMatCARS for High Energy Resolution Anomalous Scattering Instrumentation development
- 2007: NSF MRI grant ($1.4M) to Northern Illinois Univ. (S. Mini, PI) for major beamline optics upgrade
- 2007: Partnership with Exxon Mobil involving donation of equipment for proprietary access to crystallography instrumentation

Developers have ownership in the facility but are not owners. All beamtime is peer-reviewed; e. g. ASRP has a proposal review system for Australian users; ChemMatCARS has final acceptance/scheduling.

The NSF mission envelope facilitates formation of partnerships which are productive for both the facility as well as the partners.

User Statistics (thru 2007-3)

Registered Users: 416 (230 in 2005)

US

Alabama	1
Arizona	4
California	22
Colorado	7
District of Columbia	4
Florida	1
Georgia	1
Iowa	1
Illinois	115
Indiana	1
Maryland	2
Massachusetts	22
Michigan	17
Minnesota	2
Missouri	2
Montana	1
New Jersey	2
New York	33
Ohio	17
South Carolina	1
Tennessee	8
Texas	3
Virginia	1
Washington	4
Wisconsin	1

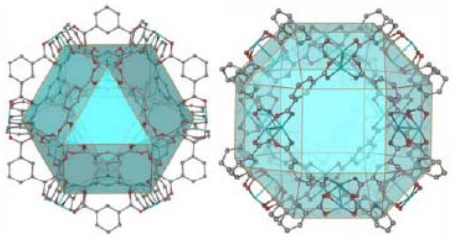
Foreign

Australia	115
Austria	1
Brazil	1
Denmark	13
Canada	1
England	2
Germany	3
Israel	1
Italy	1
Japan	1
New Zealand	1
Switzerland	2
Poland	1

ChemMatCARS hosts approximately 40 additional groups though the SCrAPS program in the US (Dr. M. Pink, Indiana Univ.) Australia (Dr. P. Turner, Univ. of Sydney)

Range of Science Program at ChemMatCARS
Sample-Driven to Collaborative Development

Service Crystallography

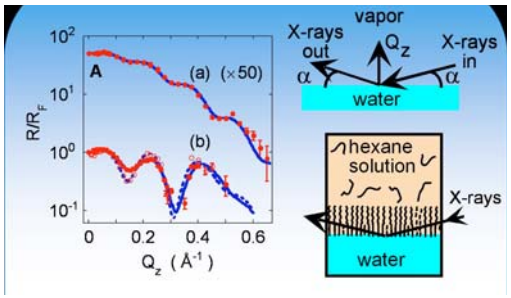


Hydrogen Storage Capacity of Metal-Organic Frameworks
Parise group SUNY Stony Brook

SAXS

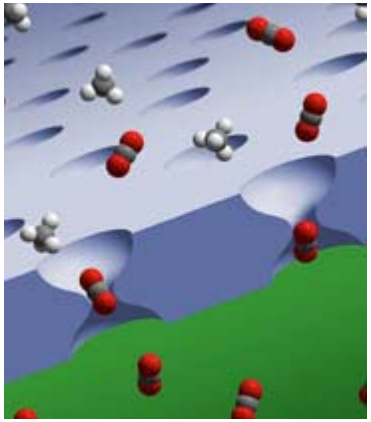
Lithium–Polymer Electrolyte Batteries
Balsara (LBL) group, **Nano Lett.** (2007)

Surface Science

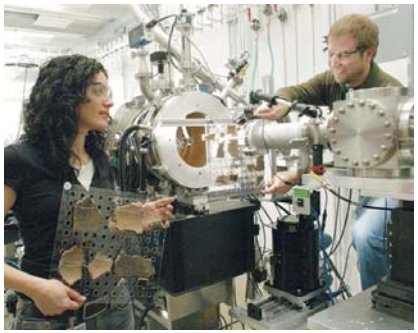


M. L. Schlossman group
U. of Illinois-Chicago "Ion Distributions near a Liquid-Liquid Interface," **Science** (2006).

SAXS



Biomimetic Polymer Membranes Park, et al., "Polymers with Cavities Tuned for Fast Selective Transport of Small Molecules and Ions," **Science** (2007). (Australian partnership)



The Social Lives of Objects: Material Culture in Ancient Eurasia
A. T. Smith, Anthropology Dept. U. of Chicago

Philip Coppens Awarded Seventh Annual IUCr Ewald Prize
"for his contributions to developing the fields of electron density determination and the crystallography of molecular excited states, ..."

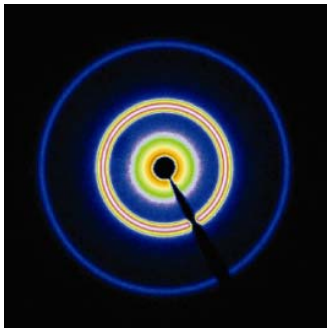
Two Examples of Facility Impact

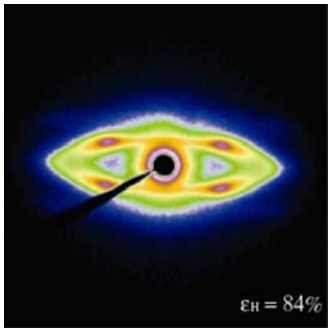
• No previous synchrotron experience:

Role of Silsesquioxane Chemistry on Structure-Property Relationships of Hybrid Polymers

Andre Lee goup, Michigan State Univ

Has succesfully competed for funding of synchrotron research. Graduate student is a candidate for a post doc position with ChemMatCARS





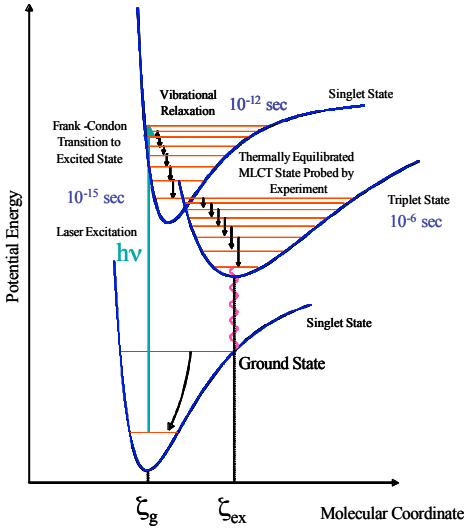
• A developer on the forefront:

A time-resolved crystallography facility at ChemMatCARS

Philip Coppens, SUNY Buffalo

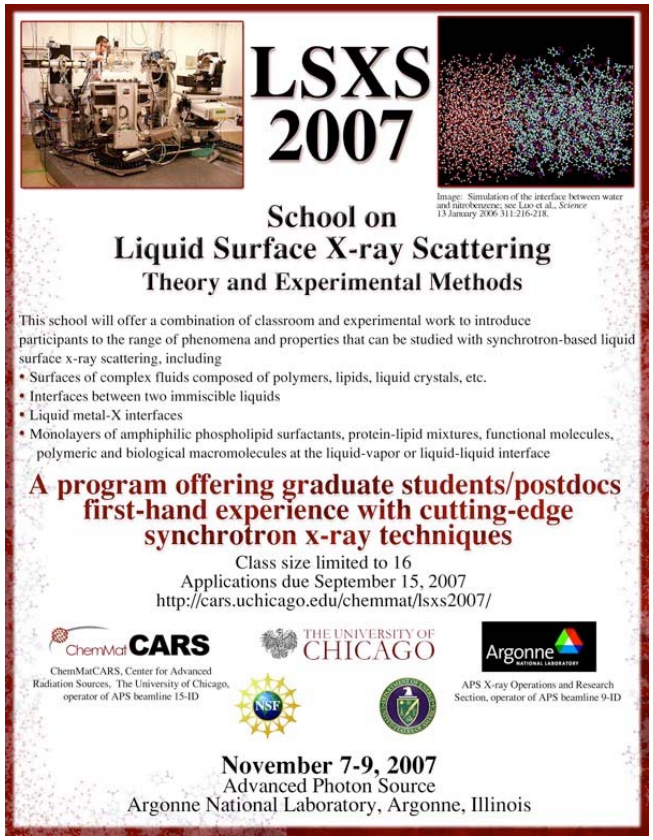
Tim Graber, ChemMatCARS

Philip Coppens pushed development of the facility.



Training

2007 School for Liquid Surface X-ray Scattering:
Theory and Experimental Methods
November 7-9, 2007
Advanced Photon Source, Argonne National Laboratory



ChemMatCARS and CARS funded the school and was responsible for arrangements, logistics, etc.

Outreach to Underrepresented Groups

- Potential scope is overwhelming for a small facility like ChemMatCARS
- ChemMatCARS is focusing on one or two “Gateways” to targeted groups

2006
Prof. Stephen C. McGuire
Department of Physics
Southern University and A&M College
Baton Rouge, Louisiana
2006 Dicussions regarding use of
x-ray standing wave technique to probe mirror microtructure
for Laser Interferometer Gravitational Wave
Observatory (LIGO) Project

2007
Prof. Edwin Walker
Department of Physics
Southern University and A&M College
Ongoing with promise
Student interns
Scientific collaboration SAXS
ChemMatCARS is part of Advisory Group for the
Proposed “Gateway” facility at the CAMD synchrotron

Challenges: Avoiding Mediocrity

- Facility must maintain a dynamic balance of
  - high throughput of users
  - high quality of scientific output
  - high quality data (good sample results in good data)
  - cutting edge experiments
- Provide high quality support, training and infrastructure to user community
- Avoid staff burn-out and enable staff professional growth
- Facility **scientific renewal** through strong, dynamic and responsive interactions with the **user community** and a strong emphasis on **training**

The community focus of NSF-funded national facilities is unique in the US and has resulted in an effective coupling of science and technology.

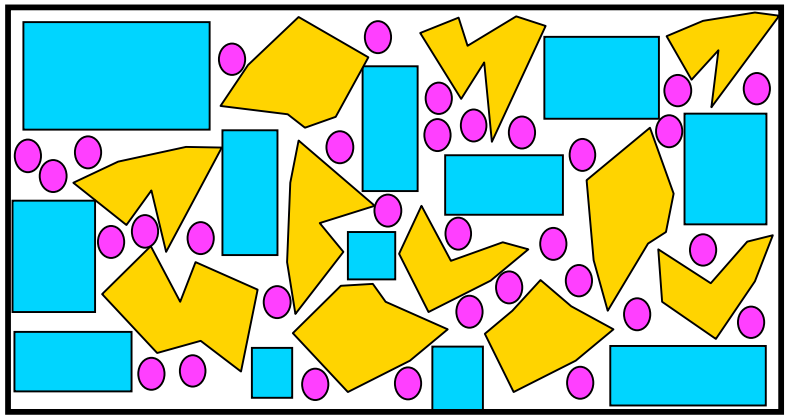
The unique environment created and ties to academic institutions greatly facilitate collaborations, community development and continual scientific renewal of the facility.

The facility is promotes cost effectiveness.

Building a ‘composite’ beam-time schedule

Aim: To pack as much science into our beam time as possible.

Finite volume in beamtime space



Cutting Edge Long lead-times required, collaborative development and technical problems can cause scheduling difficulties

Difficult Can be scheduled with certainty, but often needs lead-time

Turn **Key** Can be scheduled on short notice or regular intervals

(From the 2003 NSF/DOE ChemMatCARS Site Visit)