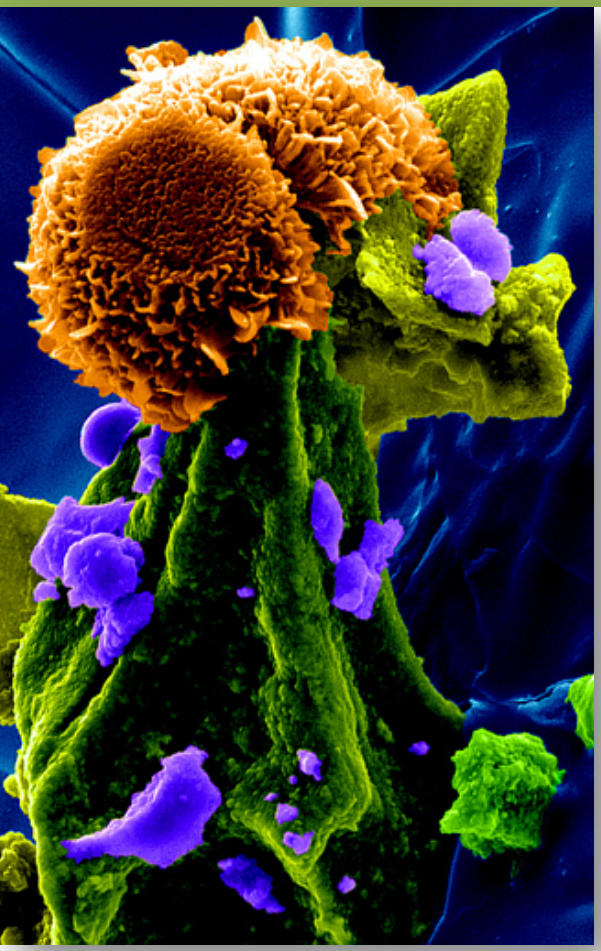
Scientific Innovation Through Integration

EMSL

EMSL Science and Capabilities – an Update to BERAC

Allison A. Campbell
EMSL Director
February 16, 2012

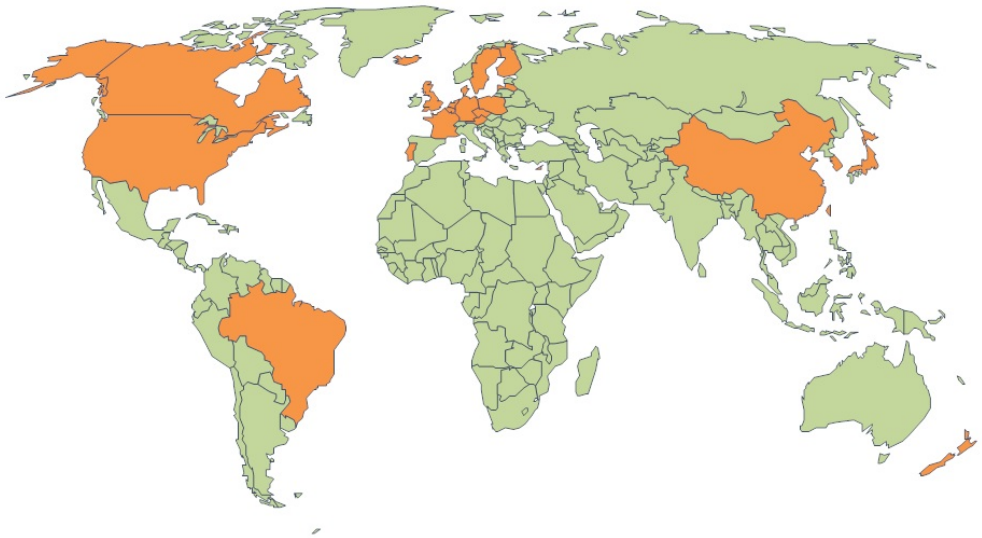
Topics for this presentation

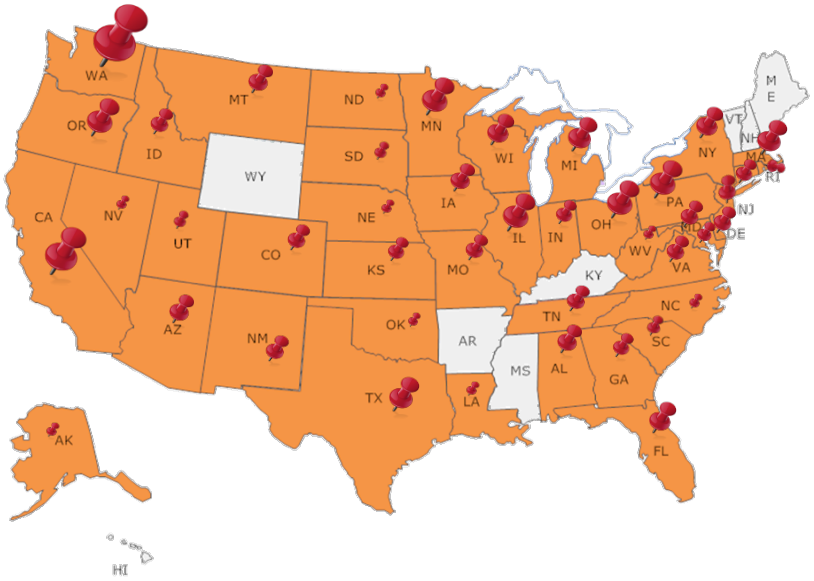


1. User statistics
2. Science themes
3. Science impact
4. New capabilities
5. Thought provoking ideas

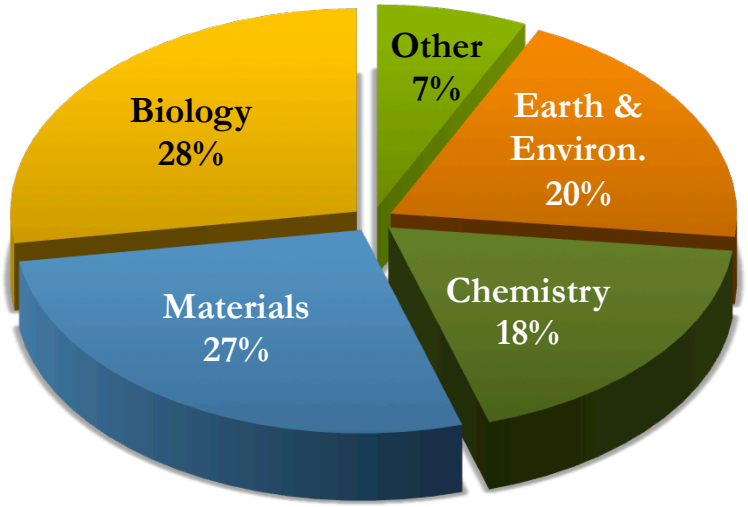
SEM Image Forsterite: EMSL users examine the interfacial reactions of olivine forsterite mineral with supercritical carbon dioxide containing water. Bruce Arey, Andy Felmy, Odeta Qafoku, Zheming Wang provided the image, which was colored by graphic designer Nathan Johnson. (BES Geosciences)

Annually over 700 scientists access EMSL through a web-based peer-reviewed proposal system

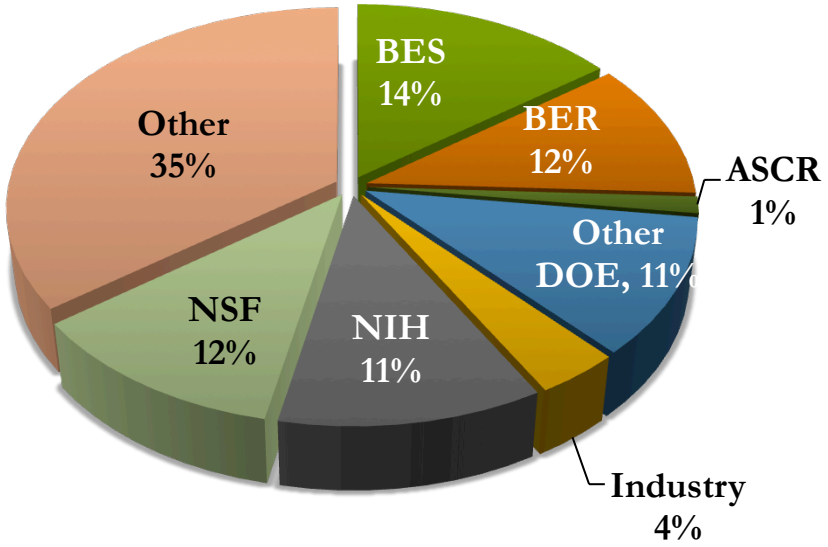




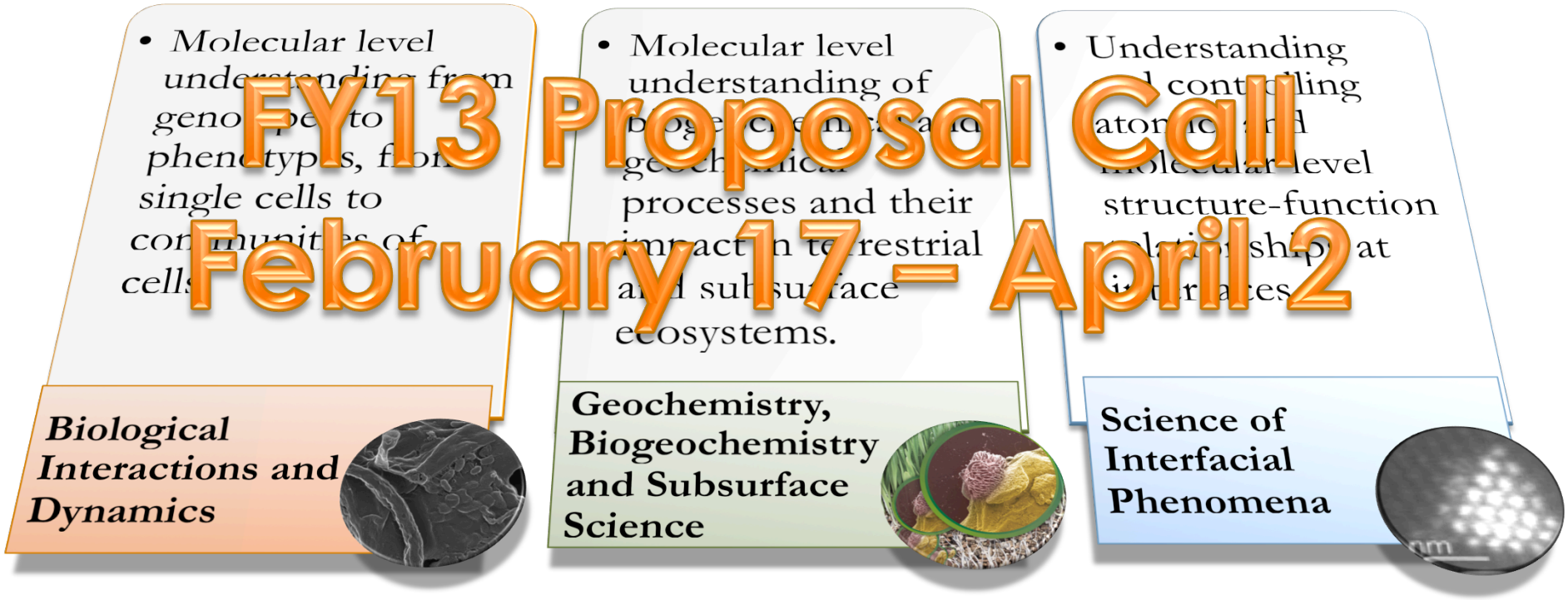
User Discipline



Funding Agency



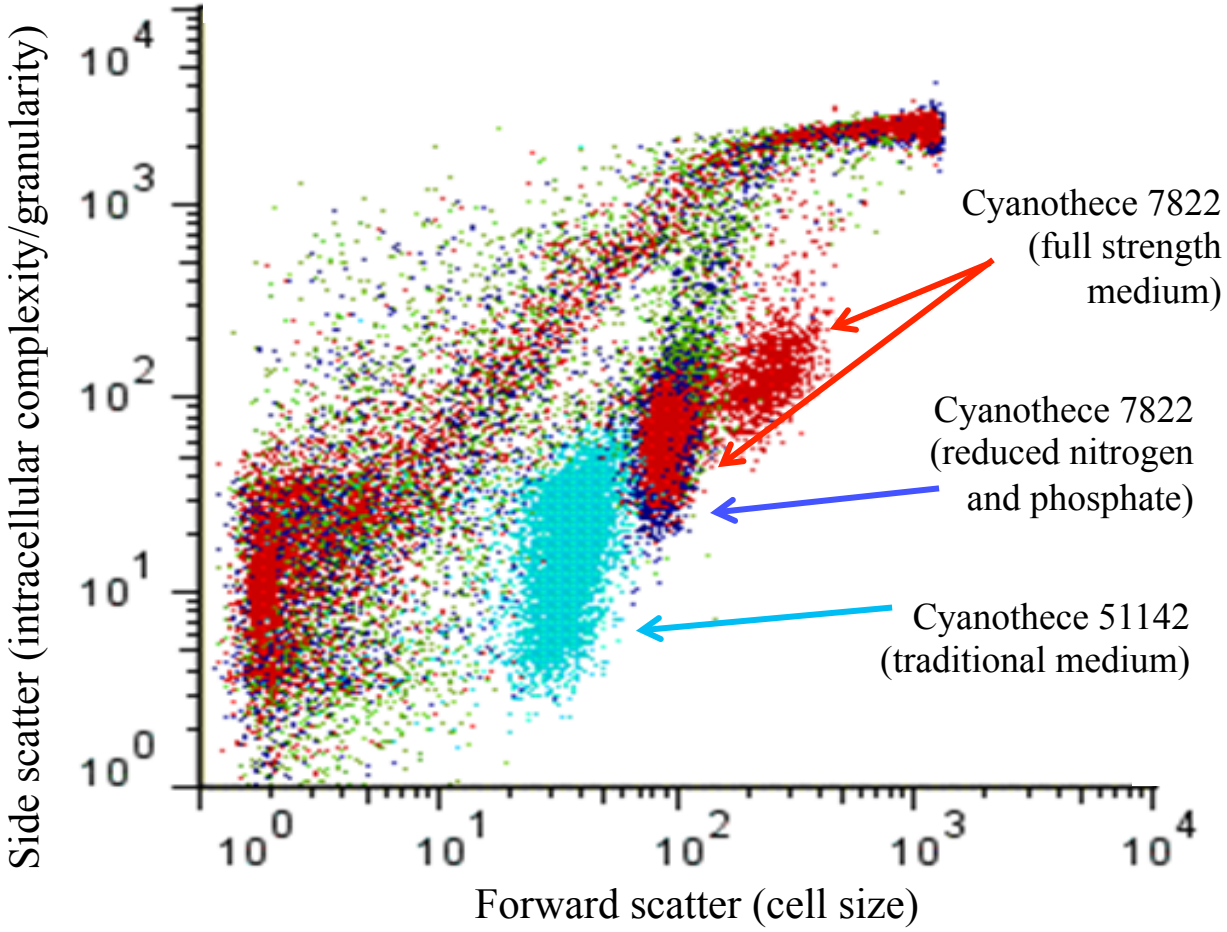
EMSL Science Themes provide the framework for proposal calls and investments



1. Build and expand upon EMSL's historical scientific expertise.
2. Align with BER and other national research programs
3. Evaluated against key criteria: relevance, user community, impact
4. Selected with broad input and support.

Systems-level model of cellular dynamics under varying conditions in cyanobacteria

Lou Sherman (Purdue) and Himadri Pakrasi (WUST);
BER GSP funded



Early results

Changes in cell characteristics observed with insight into how cell utilizes energy sources

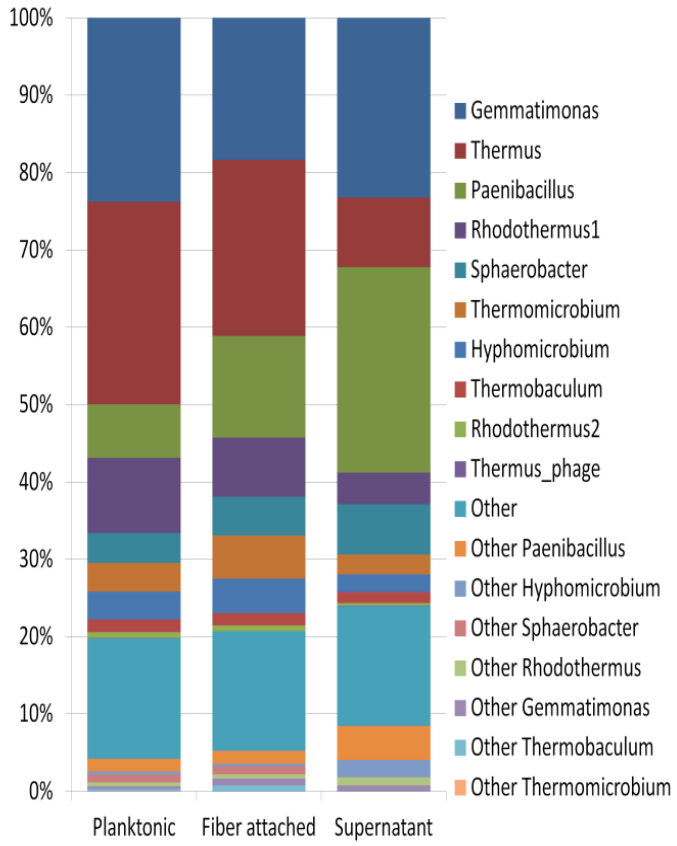
Flow cytometry & cell sorter used to analyze thousands of cells – one cell at a time

Identify genes and enzymes from thermophilic microbial communities

Steve Singer (LBNL), John Gladden (SNL), Amitha Reddy (UCD), Jean VanderGheynst (UCD), Blake Simmons (SNL); BER GSP funded

1. *Paenibacillus, Gemmatimonas* are dominant in the secretome; *Thermus* contributes surprisingly little.
2. Identified enzymes utilized during hydrolysis of treated switchgrass and better targets for development of cocktails (cellulolytic and lignolytic)
   - ✓ 29 – Glycosyl hydrolyases
   - ✓ 12 – CBM-containing proteins
   - ✓ 9 – Oxidoreductases
   - ✓ 3 – Possible H-bonding disruptors

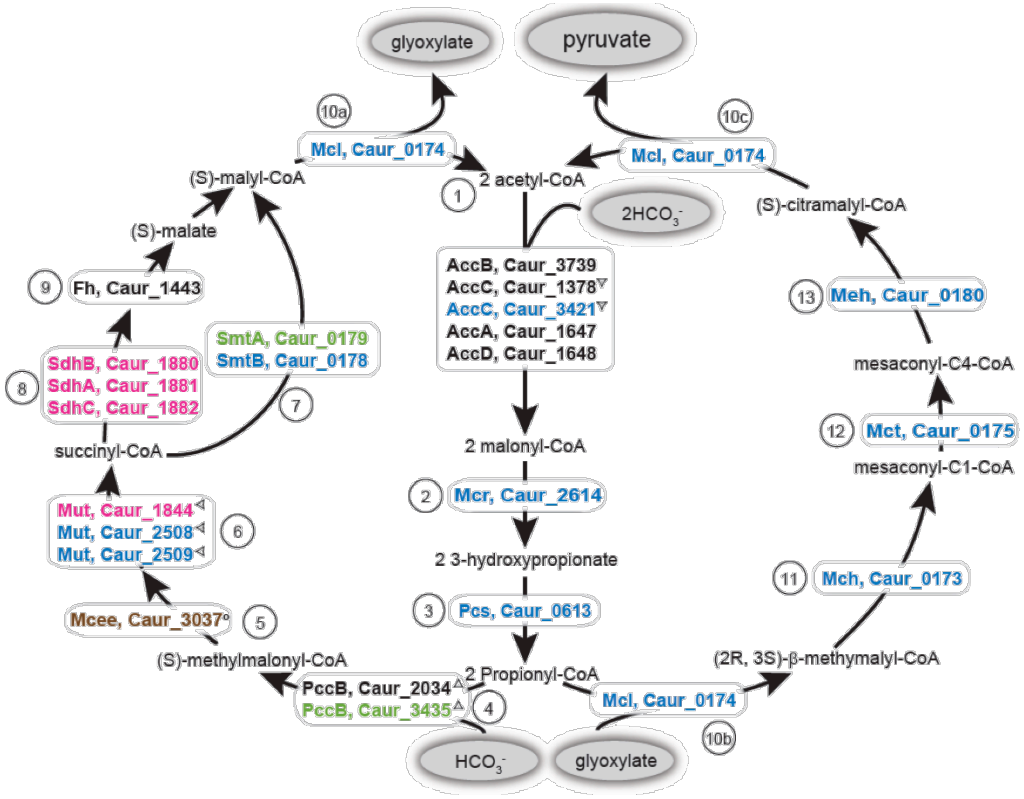
Abundance of metagenome bins in proteome (by AMT):



Gaining a better understanding of carbon uptake and energy transformation through anoxygenic photosynthesis

Li Cao (PNNL), Donald A. Bryant (PSU), Athena A. Schepmoes (PNNL), Kajetan Vogl (PSU), Richard D. Smith (PNNL), Mary S. Lipton (PNNL), Stephen J. Callister (PNNL); BER GSP and BES funded

Proteomics identified proteins relevant to anoxygenic photosynthesis in *C. aurantiacus*, a model anoxygenic phototroph having the 3-OHP carbon fixation pathway



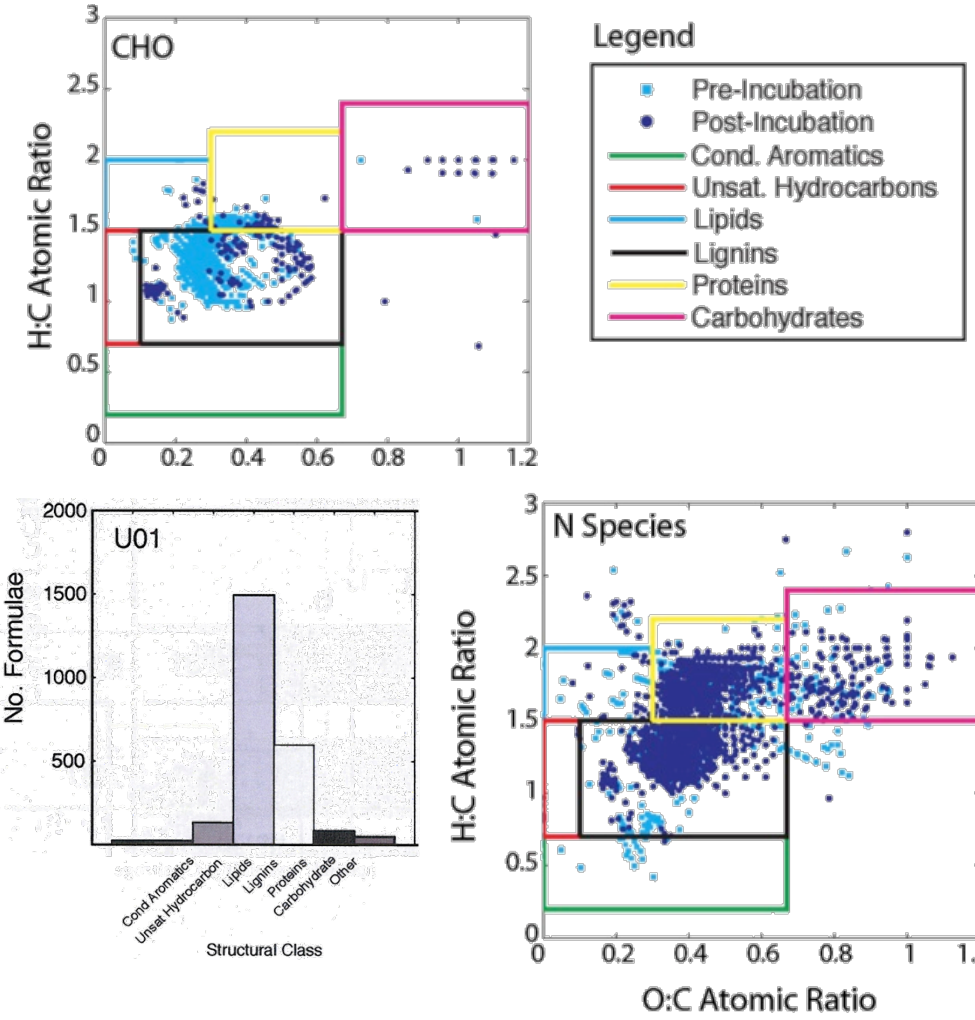
3-OHP carbon fixation pathway for *C. aurantiacus*. Proteins in blue/green were observed in greater abundance/ uniquely during anoxic growth.

L Cao et al. *Photosynthesis Research* (2012) 110(3), 153-168

Understanding biogeochemical processes driven by naturally occurring organic material in a U-contaminated aquifer (Rifle IFCR)

Paula J. Mouser (OSU), Michael Wilkins (PNNL), Don Smith (AMOLF), Kenneth Williams, (LBNL), Ljiljana Pasa-Tolic (EMSL), and Philip Long (LBNL)

1. Microbial activity and associated redox processes are influenced by both the availability and form of dissolved organic matter.
2. FTICR MS with ESI is effective in elucidating molecular-scale differences in DOM from complex environments where nutrients may effect both microbial activity and contaminant mobility.



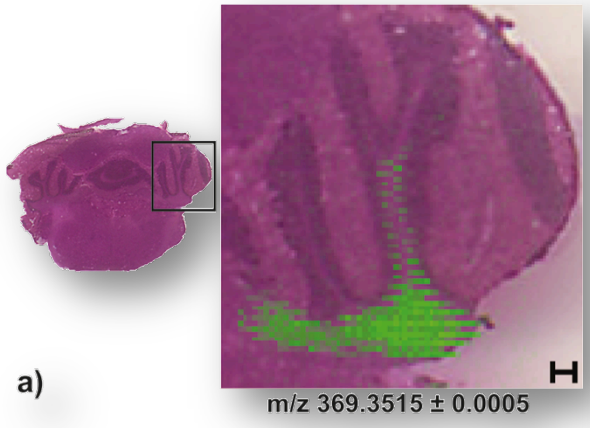
EMSL's C_{60} SIMS FTICR MS raises bar for mass accuracy, resolving power

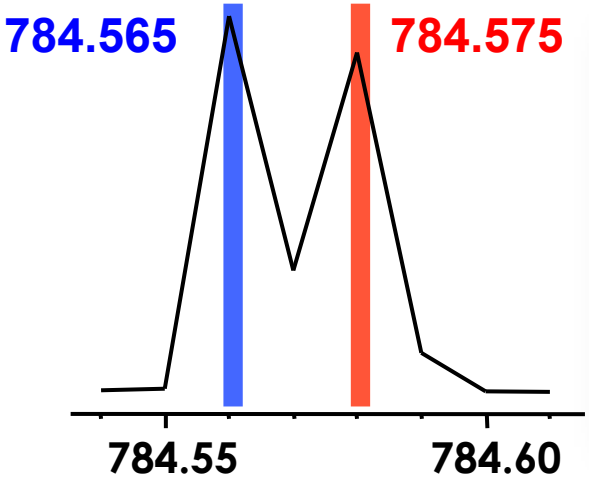
Don Smith (AMOLF), Robby Robinson (EMSL), Aleksey Tolmachev (EMSL), Ron Heeren (AMOLF), and Ljiljana Pasa-Tolic (EMSL).

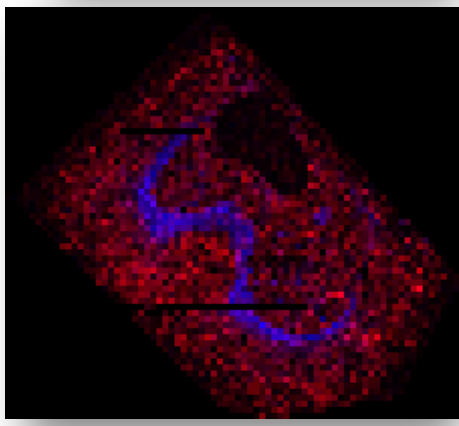
- Molecular location dictates much about how biological system function
- High-resolution mass spectrometry enables scientist to locate and identify biomolecules with higher mass accuracy and mass resolution than ever before.
- Couples C_{60} ionization with the high spatial resolution of SIMS and high mass resolution of FTICR MS.

Demonstrated the potential of C_{60} SIMS FTICR MS using mouse brain tissue.

- Achieved mass accuracy and mass resolving power 10 times higher than previously reported for SIMS.
- Optimizations are underway for achieving sub-micrometer resolution and building advanced data handling and analysis tools.







X-ray computed tomography and microfluidics enable pore structure visualization in natural systems

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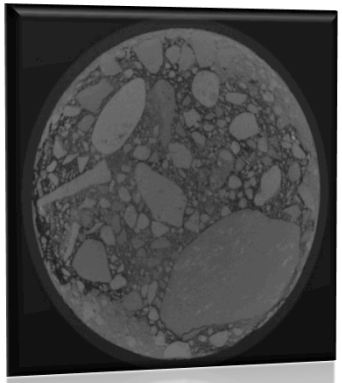

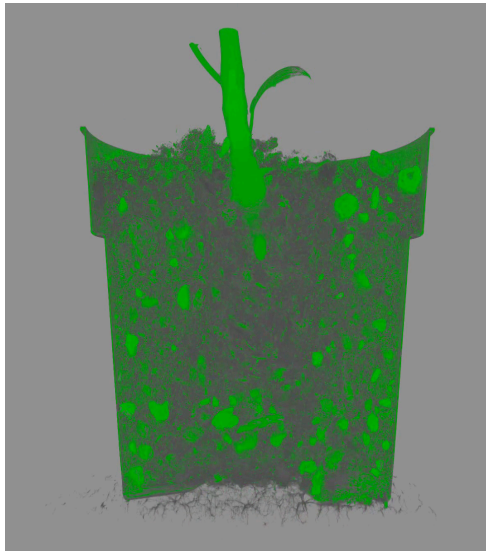

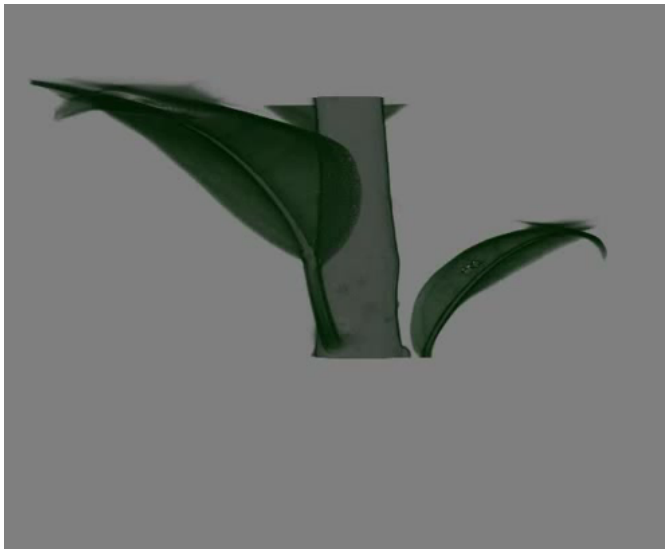

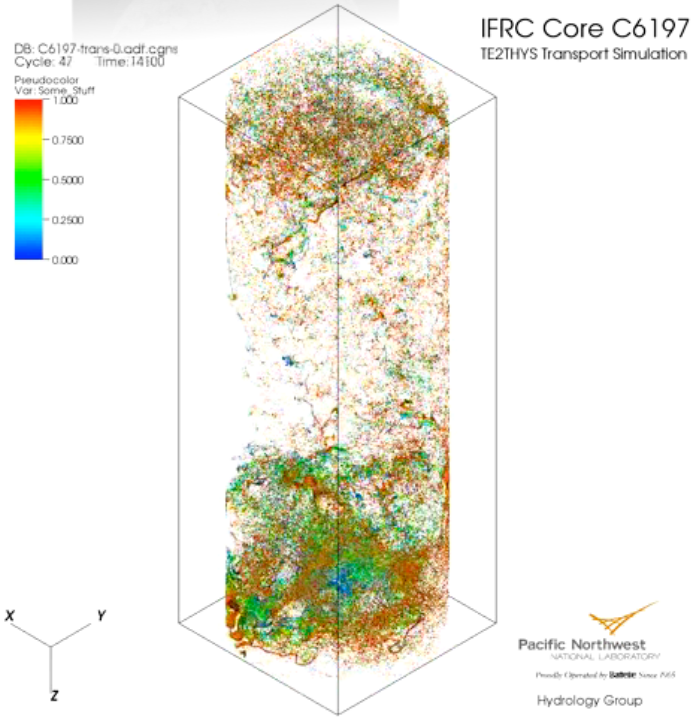

IFRC Core C6197

TE2THYS Transport Simulation

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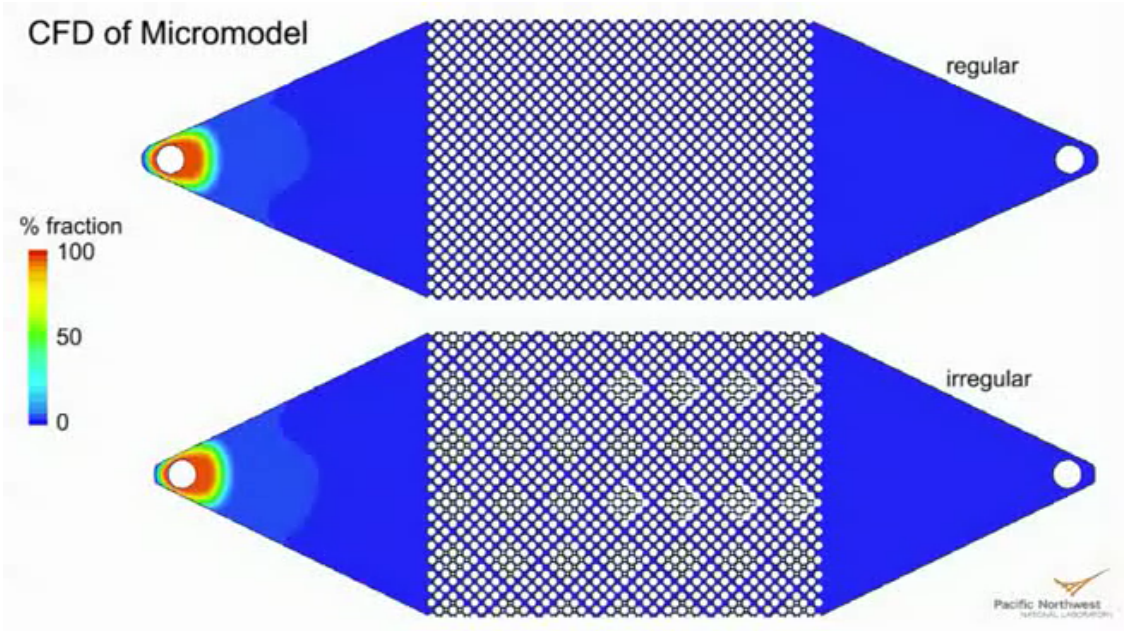
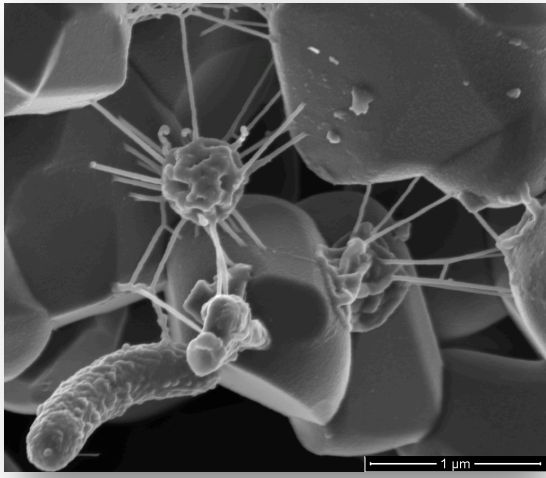
Hydrology Group



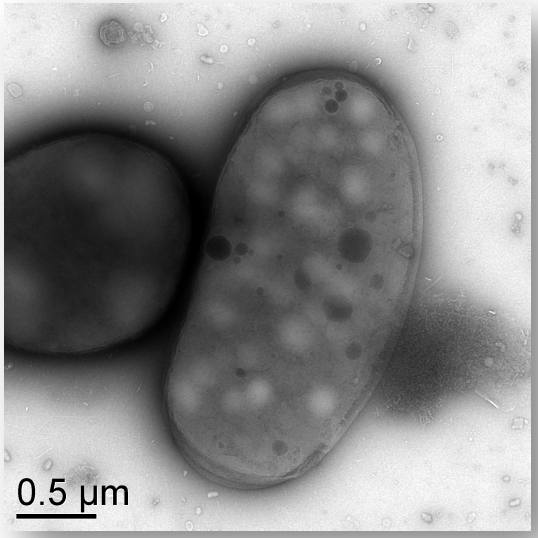
New Quiet wing brings new science opportunities

- 2 Aberration corrected TEM's
  - 1 Environmental (temperature, controlled atmosphere)
- Helium ion microscope
- 2 Ultra high vacuum STM's
- TEM for biological samples
- Dynamic TEM

HeIM image: Shewanella on SiO_2; John Zachara (PNNL)



TEM image of bacteria from a hot lake biofilm which has extremely large carbonate content. Jim Fredrickson (PNNL) is investigating the role that these bacteria have in the CO_2 fixation process.



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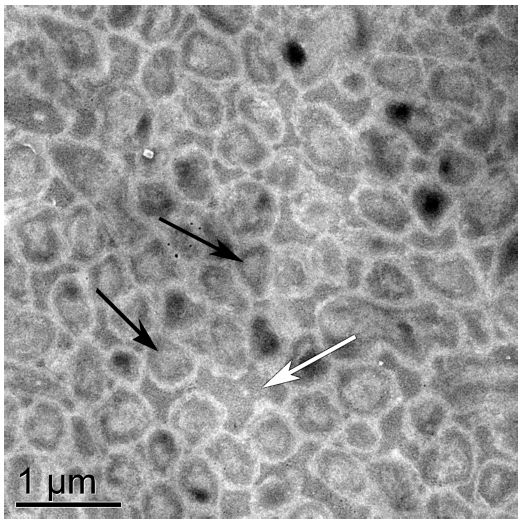
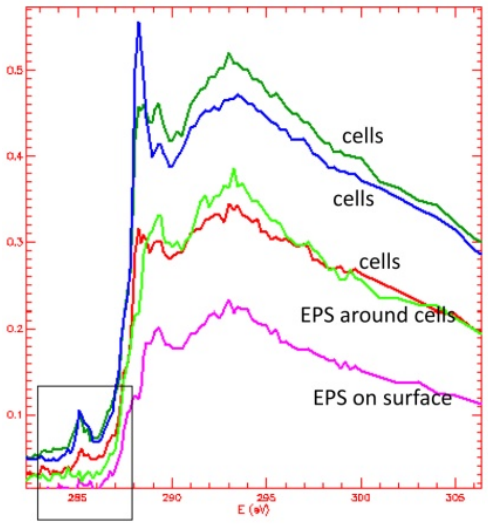
Constructing a spatially resolved correlative chemical map of biofilm interactions with metal ions

Matthew J. Marshall (PNNL) BER SBR Early Career Award



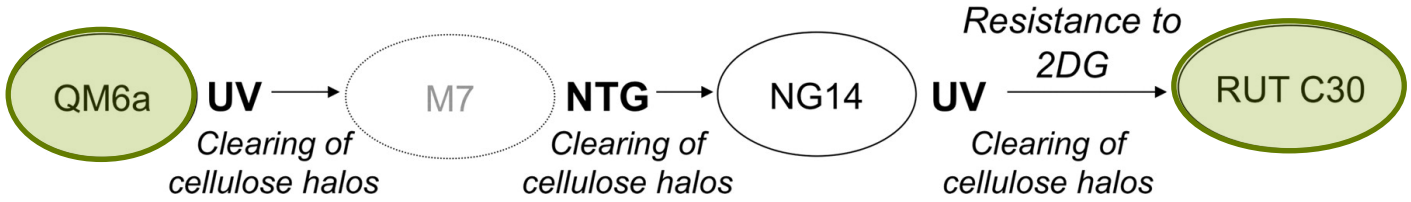


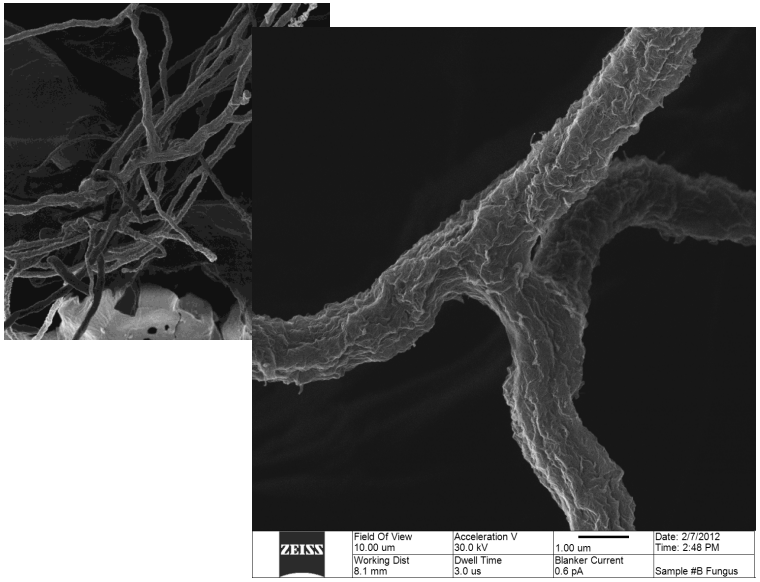
TEM image of *Shewanella* biofilm showing dense packaging of cells (black arrows) in extracellular polymeric substance (EPS) matrix (white arrow). Cells were prepared by cryo-sectioning and imaged at room temperature at EMSL, followed by Scanning Transmission X-ray Microscopy (STXM) chemical imaging of carbon at the ALS, sector 5.3.2.1. Matthew Marshall and Alice Dohnalkova at PNNL with David Kilcoyne at the ALS

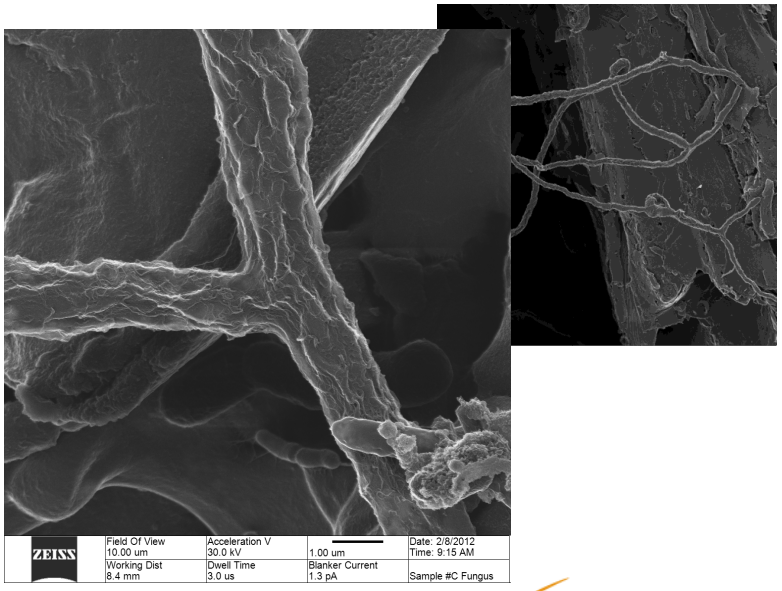
- Goal - Understand the physical and chemical interactions of hydrated biofilms and catalytic components of EPS as they interact with redox active metal ions and influence biogeochemical reactions.
- Construct 3D renditions of biofilm EPS interacting with metal ions based upon cryoTEM, µXRF, nanoSIMS and STXM analysis.

HeIM reveals new phenotypes in *Trichoderma reesei*

Increased cellulase production; decreased catabolite repression







Genomics: Le Crom S et al. PNAS 2009;106:16151-16156
EMSL Microscopy: Bruce Arey and Alice Dohnalkova, Sue Karagiosis and Scott Baker (EERE funded)

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Pushing the frontiers of microscopy – *in situ* dynamic measurements

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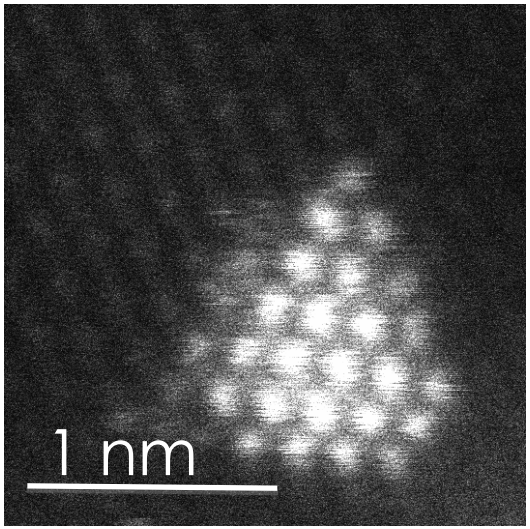
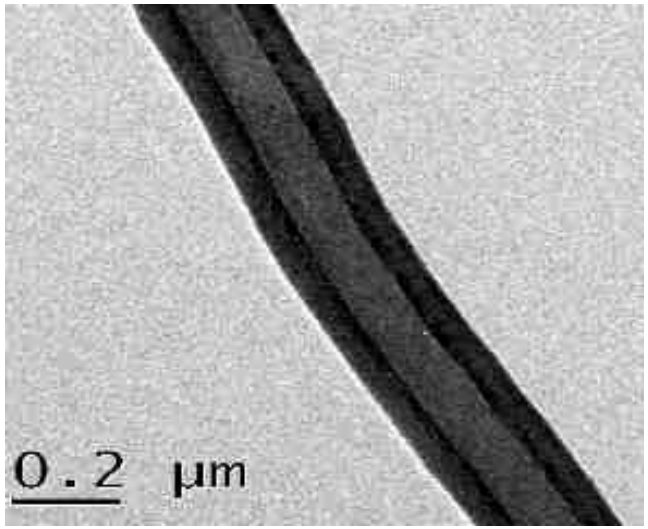
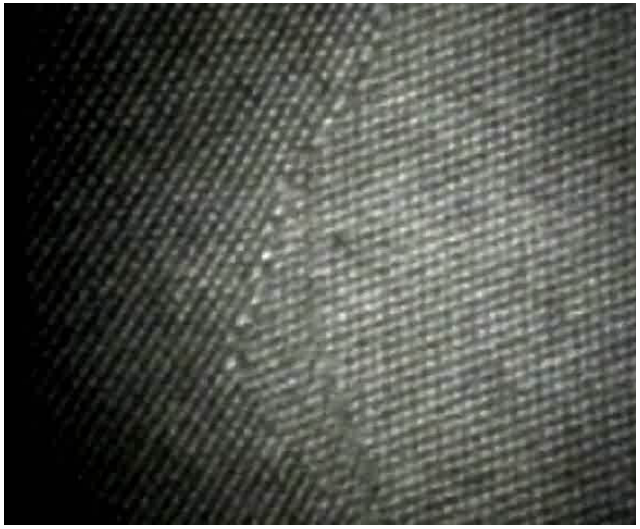
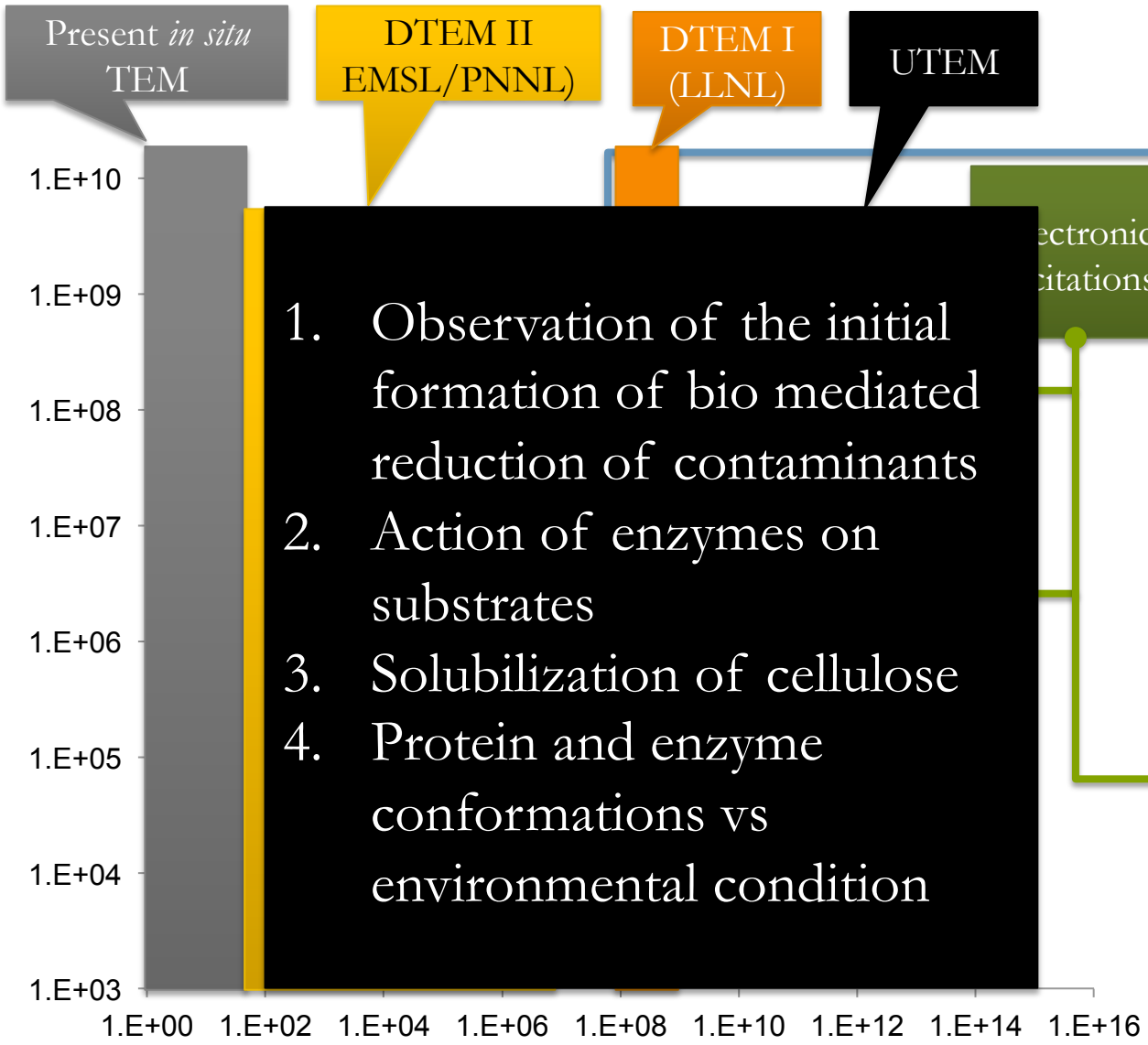
High Resolution	In situ, dynamic	High resolution, dynamic
		
Angstrom resolution Static	Micron resolution 80 fps	Nanometer resolution Microsecond
Ir on $MgAl_2O_4$ L. Kovar (EMSL) EMSL Titan	Li diffusion in Si on CNT C. Wang (EMSL) EMSL Titan	Grain Boundaries in Au K. Merkle (ANL) ARM Stuttgart, Germany

The potential of time resolved *In-Situ* TEM



1. Observation of the initial formation of bio mediated reduction of contaminants
2. Action of enzymes on substrates
3. Solubilization of cellulose
4. Protein and enzyme conformations vs environmental condition

Biology

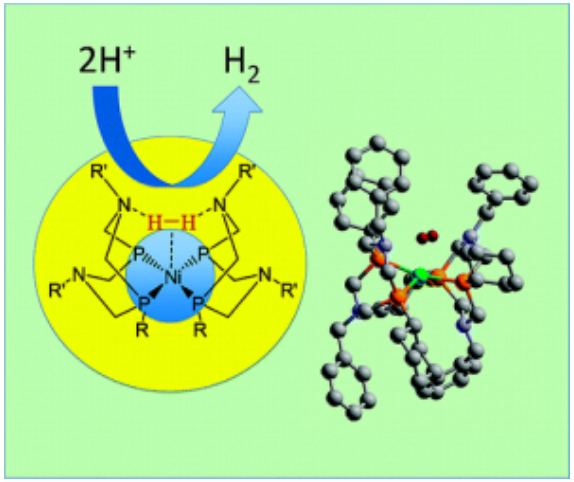
- Protein dynamics
- Cellular interactions
- Molecular processes in cell and at membranes

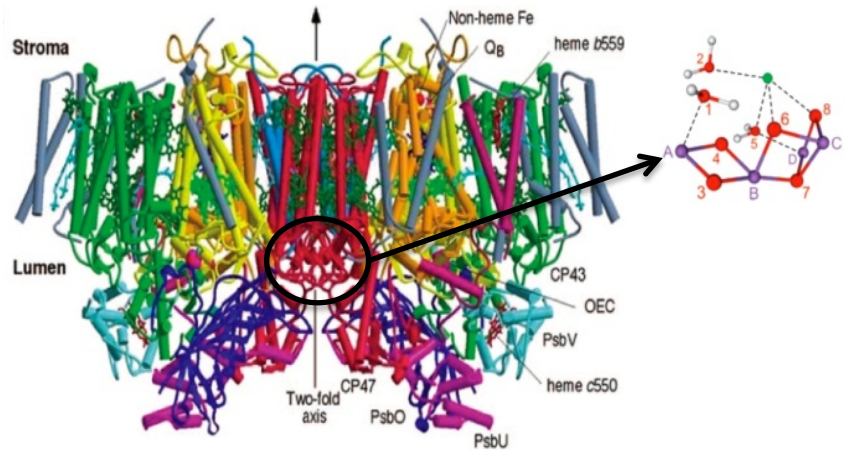
Biogeochemistry

- Phase transformation
- Electron transfer
- Bond breaking/ forming

Next generation magnetic resonance spectrometry (under consideration)

- Need better understanding of interplay of oxidation state on structure for many biological complexes (ie Photosystem II, catalytic reaction sites)
- Multi-modal, real-time probing of electronic and nuclear spins is required
- Next-gen NMR, DNP, EPR system is envisioned and planned (workshop December 2011)

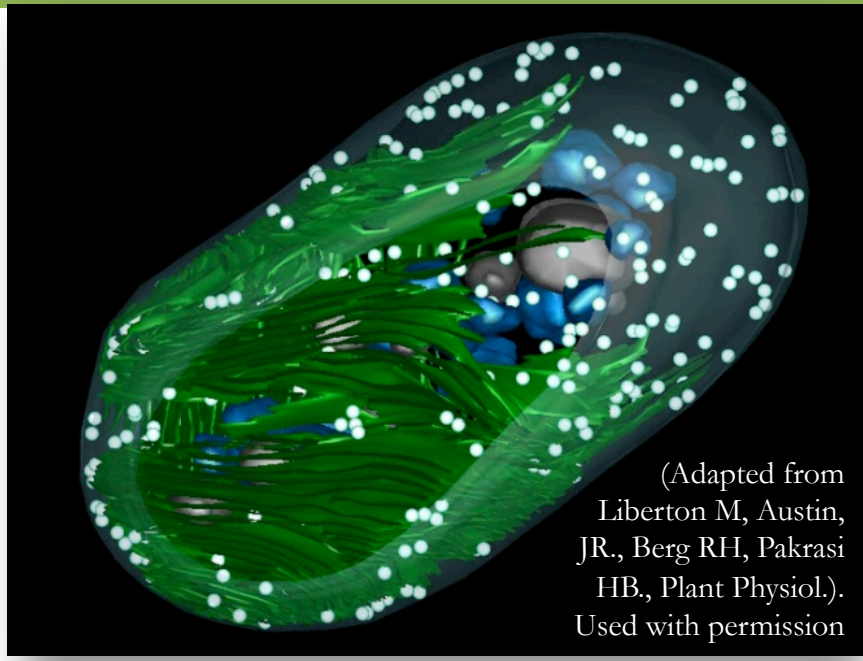




Biosystems cartography at single cell and subcellular resolutions

Goals:

1. A census of cells from homogenous or mixed populations.
2. At subcellular resolution, understand, model and manipulate populations of individual cells.
3. Acceleration of research in systems and synthetic biology for production of biofuels and renewable chemicals, global carbon cycling, plant science and complex microbial communities.

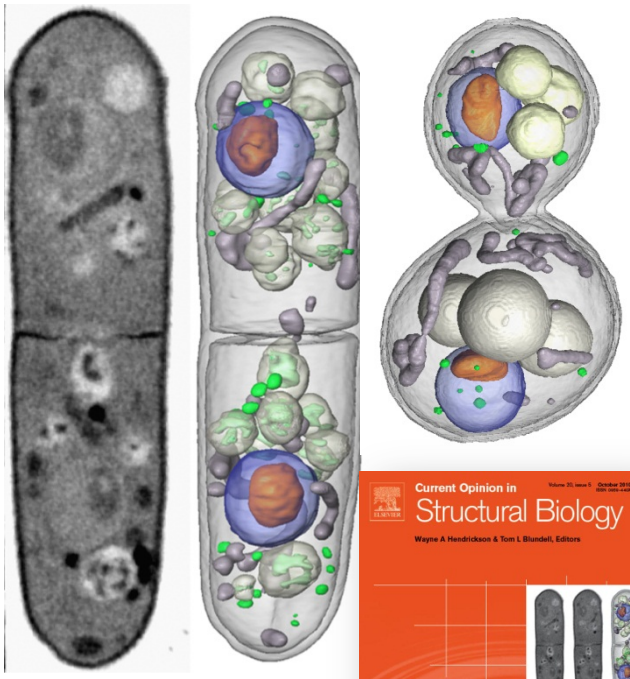


(Adapted from Liberton M, Austin, JR., Berg RH, Pakrasi HB., Plant Physiol.). Used with permission

- Integrated -omic measurements with single cells resolution
- Advanced cell sorting techniques
- Advanced microscopy
- Model driven data integration (Data integration, molecular modeling and simulation)

We are exploring the possibility of a compact x-ray light source at PNNL/EMSL

- Combining EMSL's expertise and capabilities with an in-house X-ray facility (like a Compact X-Ray Light Source - CXLS) will enable us to achieve an unprecedented level of multi-modal characterization.
- The pulse width of a CXLS will be 10 - 300 fsec. This is ideally suited for time-resolved studies on real systems (e.g.: life times and fate of charge carriers). But will have a sufficiently high brightness to allow dynamic imaging experiments.
- Biological materials are sensitive to radiation damage under interrogation. A CXLS can provide X-rays with lower photon density per pulse thereby limiting radiation damage.



Yeast organelle structure
C. Larabell, UCSF/LBNL
With permission.

Workshop held Sept. 2011 to discuss the science impact this room-sized capability could have on achieving multi-modal chemical imaging of chemical, biological, environmental and materials science challenges

Questions?

EMSL

Environmental Molecular Sciences Laboratory

Allison A. Campbell, Ph.D.
Associate Laboratory Director

902 Battelle Boulevard
P.O. Box 999, K8-84
Richland, WA 99352
www.emsl.pnl.gov

Tel: (509) 371-6000
Fax: (509) 371-6072
allison.campbell@pnl.gov