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Pacific Northwest NATIONAL LABORATORY
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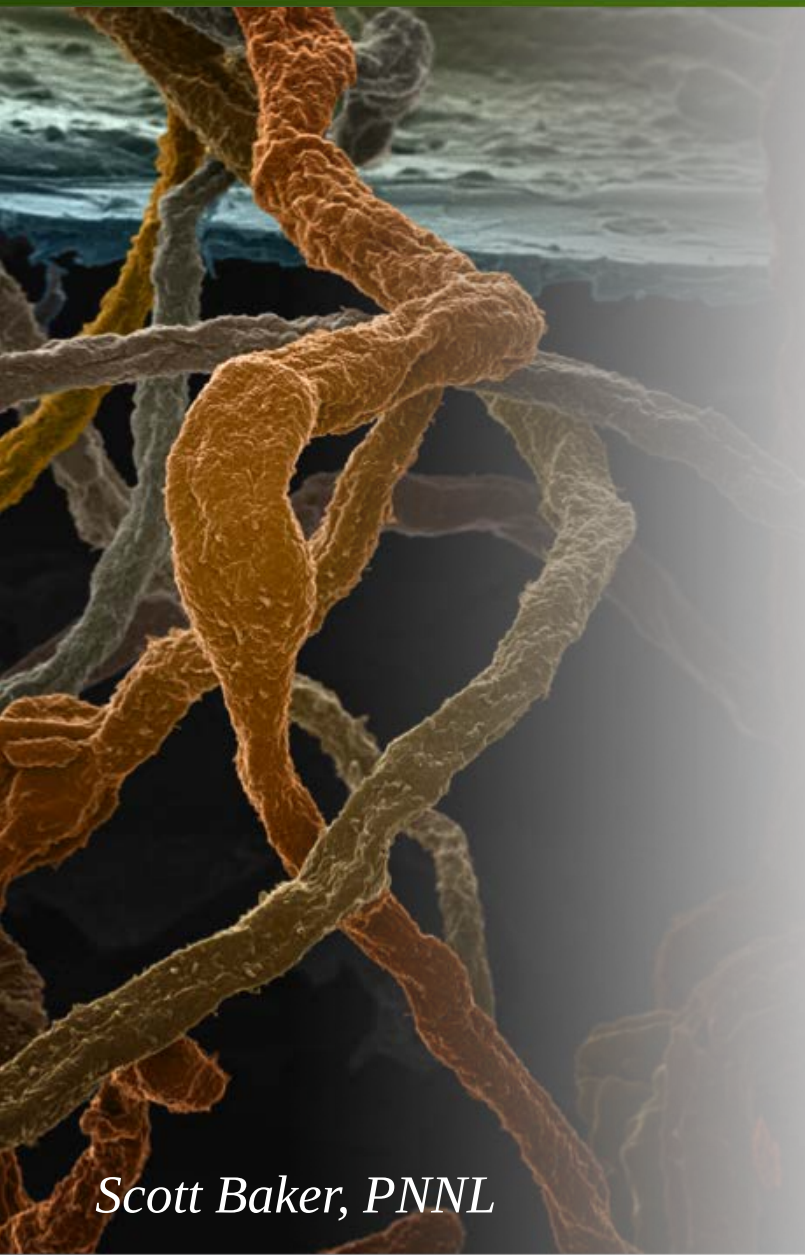
U.S. DEPARTMENT OF ENERGY

EMSL Update:
Science Themes, Capabilities and the User Program

Allison A. Campbell
EMSL Associate Laboratory Director

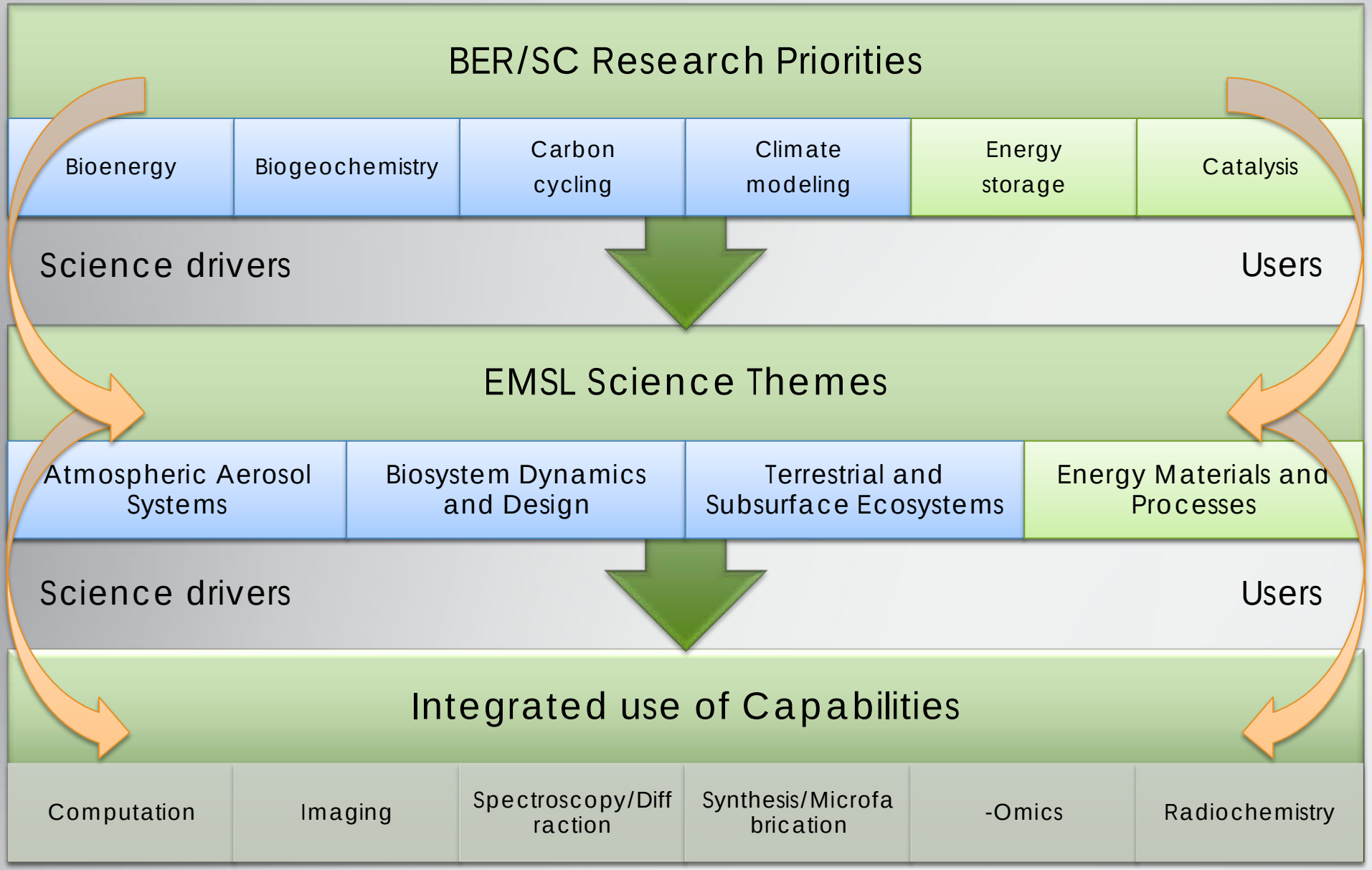
March 4, 2014

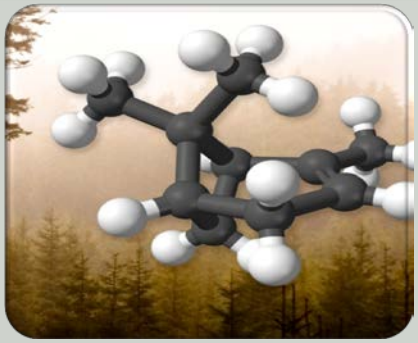
Today's topics

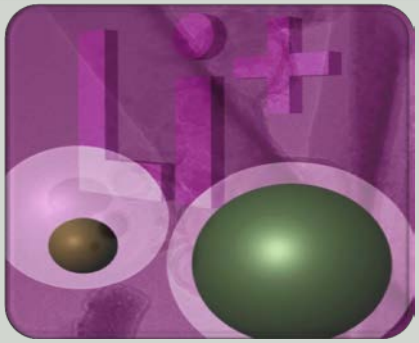


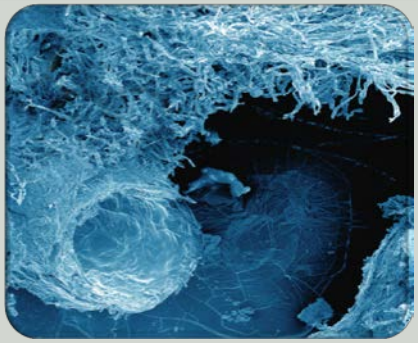
Scott Baker, PNNL

- Science
- Capabilities
- Outreach
- Users


BER/SC Research Priorities
Bioenergy
Biogeochemistry
Carbon cycling
Climate modeling
Energy storage
Catalysis
Science drivers
Users
EMSL Science Themes
Atmospheric Aerosol Systems
Biosystem Dynamics and Design
Terrestrial and Subsurface Ecosystems
Energy Materials and Processes
Science drivers
Users
Integrated use of Capabilities
Computation
Imaging
Spectroscopy/Diffraction
Synthesis/Microfabrication
-Omics
Radiochemistry







ATMOSPHERIC AEROSOL SYSTEMS

BIOSYSTEM DYNAMICS & DESIGN

ENERGY MATERIALS & PROCESSES

TERRESTRIAL & SUBSURFACE ECOSYSTEMS

Coupling across spatial and temporal scales

Informing models for improved prediction and control of complex systems

1. **Evaluated** against key criteria: Impact, alignment, user community
2. **Developed** with input from Advisory groups, users and stakeholders
3. **Used** as the basis for proposal calls and investments

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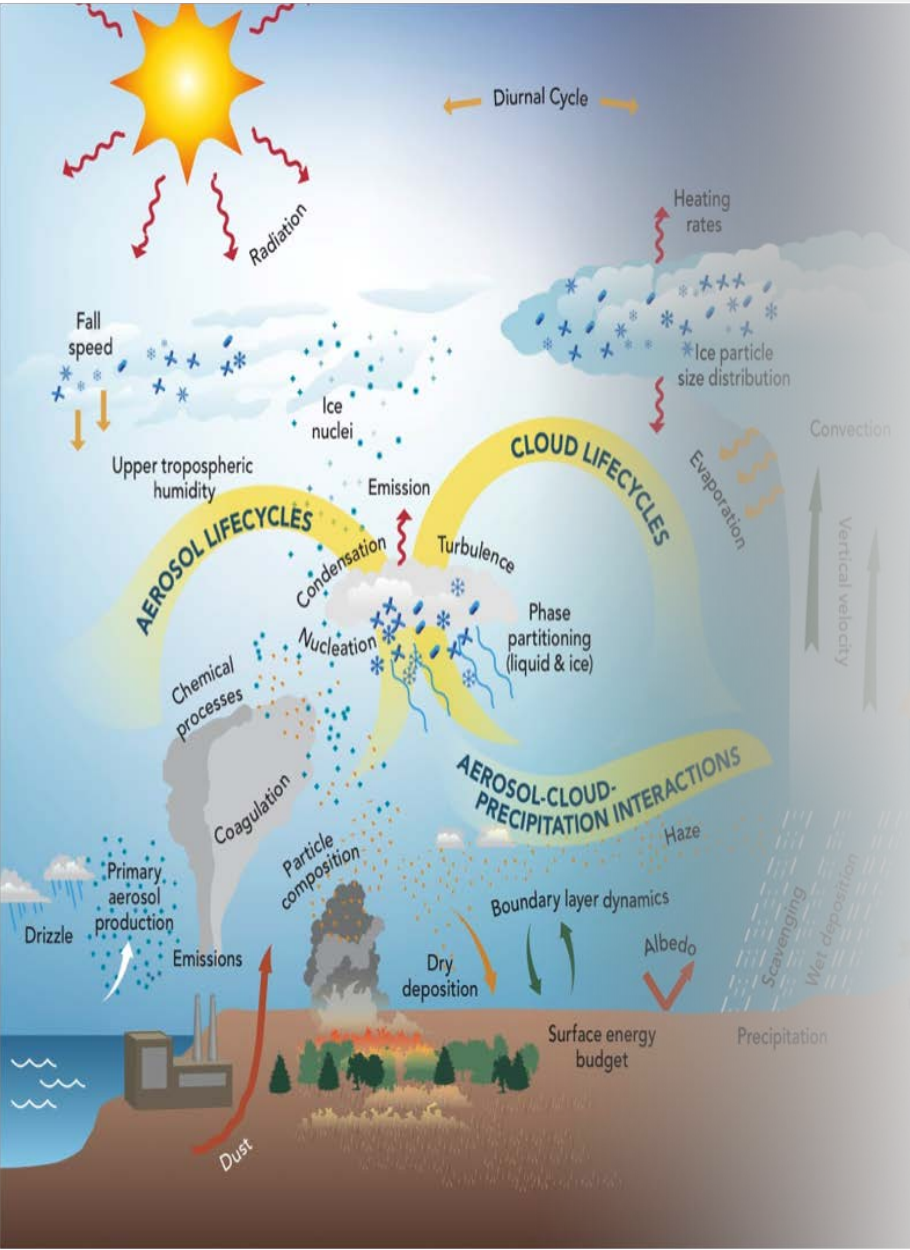
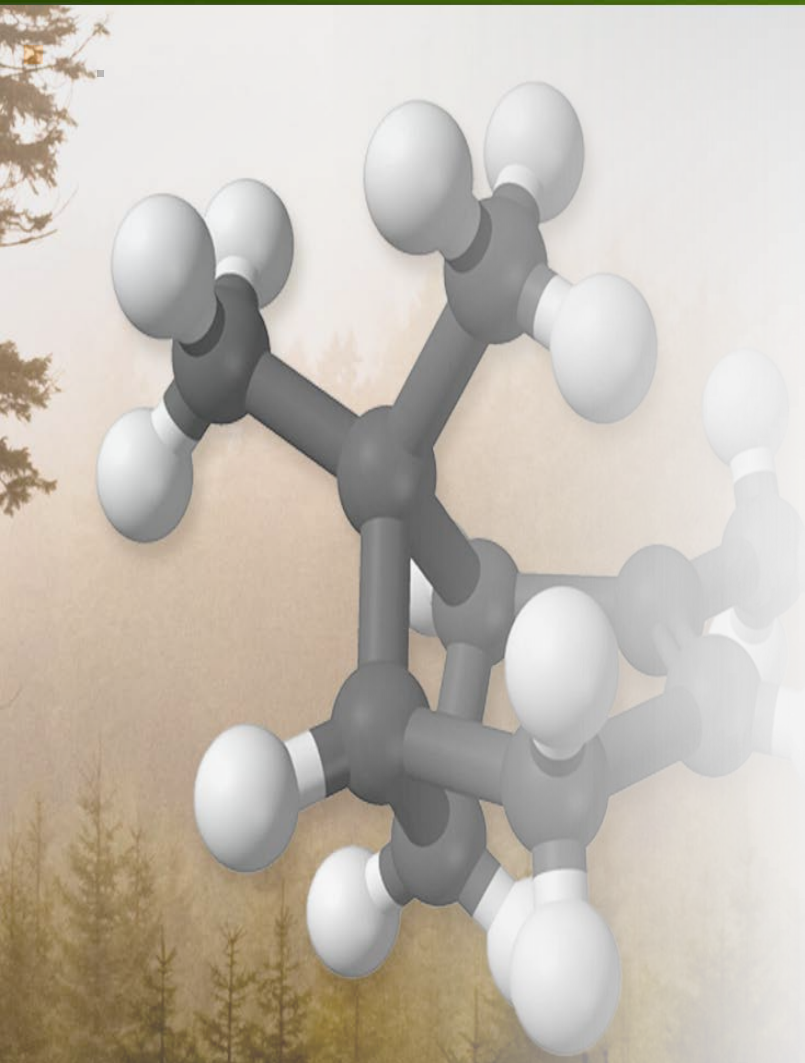
Atmospheric Aerosol Systems



Our focus: Understanding molecular-scale dynamics of aerosols to improve climate model simulations and enable predictive understanding.

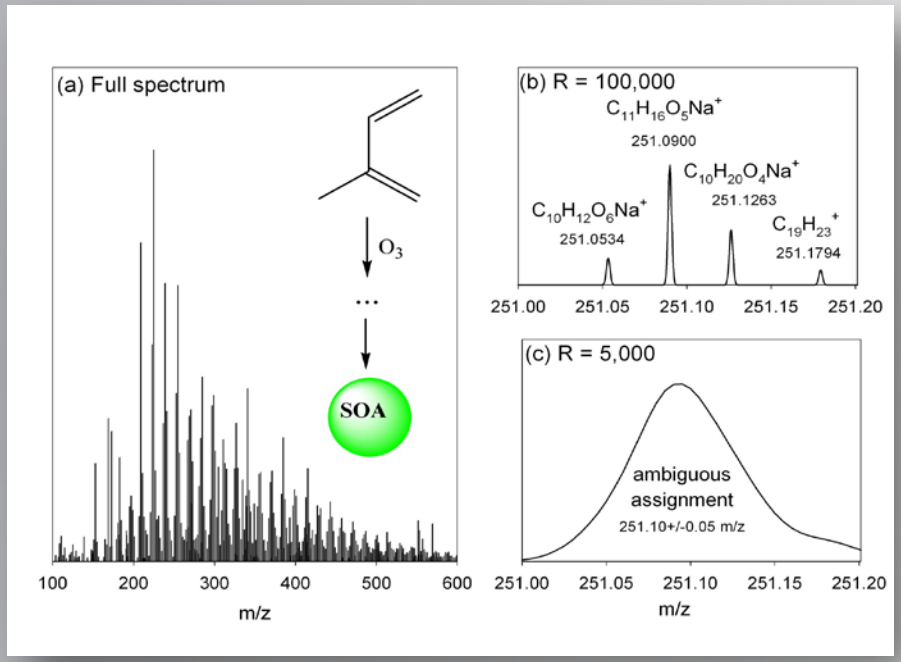
Special interest – Biogenic organic aerosols.

Biogenic organic aerosols: A key component in aerosol-cloud-precipitation-radiation processes



10-year Goal: Understand the molecular scale processes that enhance the formation of biogenic volatiles and determine the radiative properties of OA to improve the accuracy of climate model simulations.

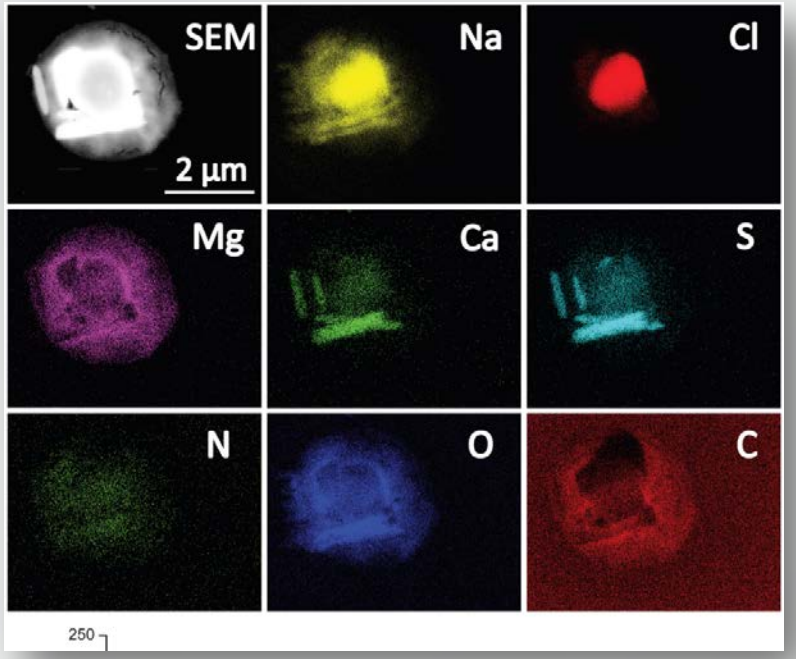
Laboratory chamber studies of BOA formation



Nguyen et al. Atm. Environ. 44 (2010) 1032-1042

Field studies of anthropogenic pollution impacts on BOA formation:

CARES study



Zaveri et al. *Atmos. Chem. Phys.*, 2012

Laskin et al. 2012

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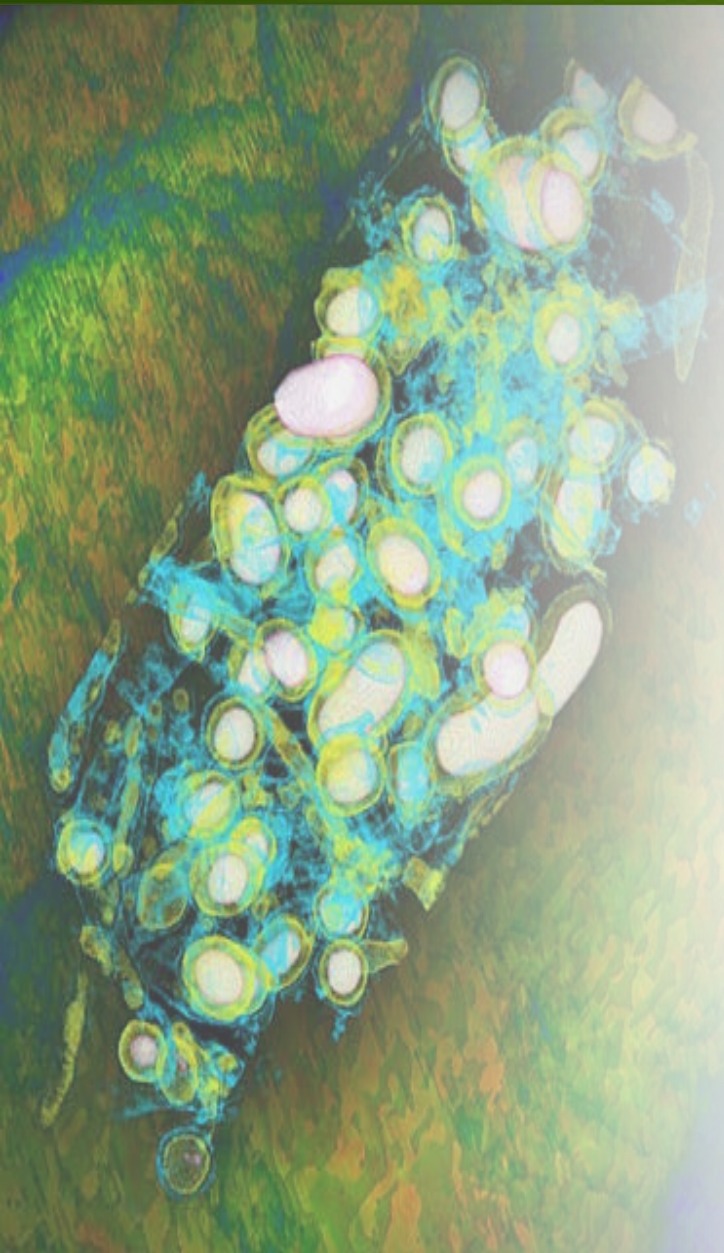
EMSL links to BER campaigns

EMSL's Liz Alexander (left) and Suzane Simones, a Harvard University graduate student investigate the GOAmazon T3 research site near Manacapuru, Amazonia

- EMSL is excited to be part of current GO Amazon campaign
  - Deployed staff and mass spectrometers

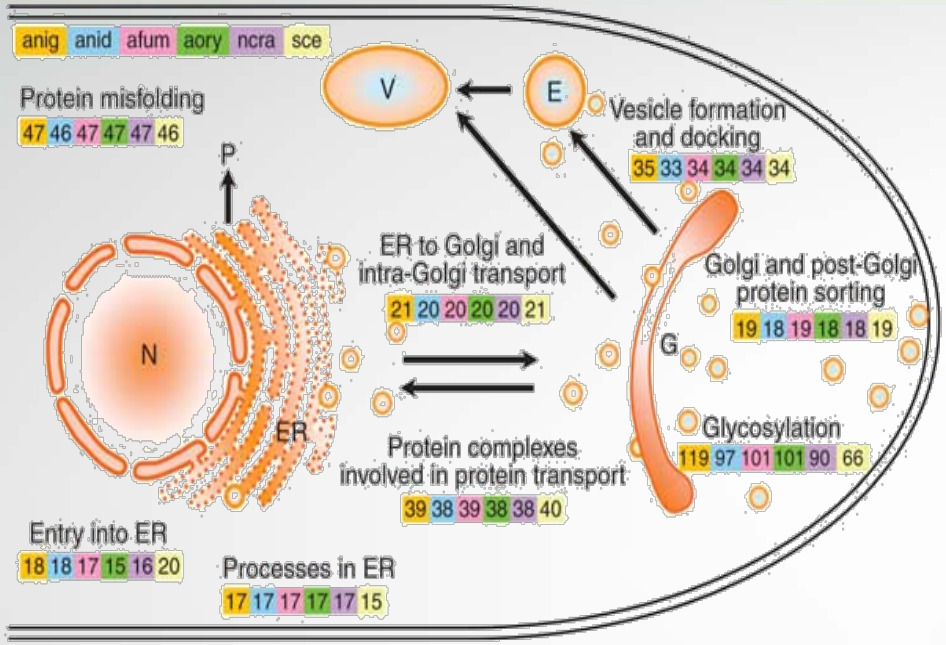
Biosystem Dynamics and Design



Our focus: Understanding biological processes (from individuals to communities) in time and space.

Special interest: Metabolic compartmentalization.

Compartmentalization: Understanding the cell factory

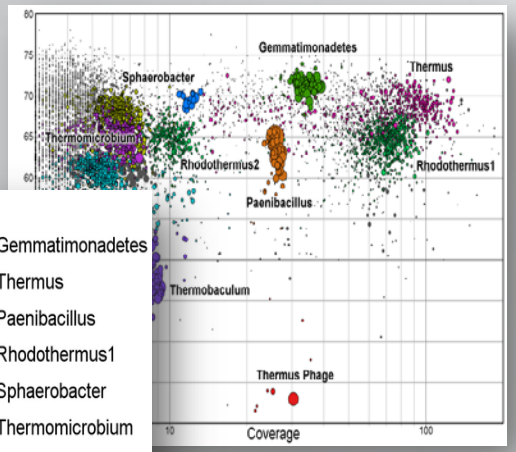


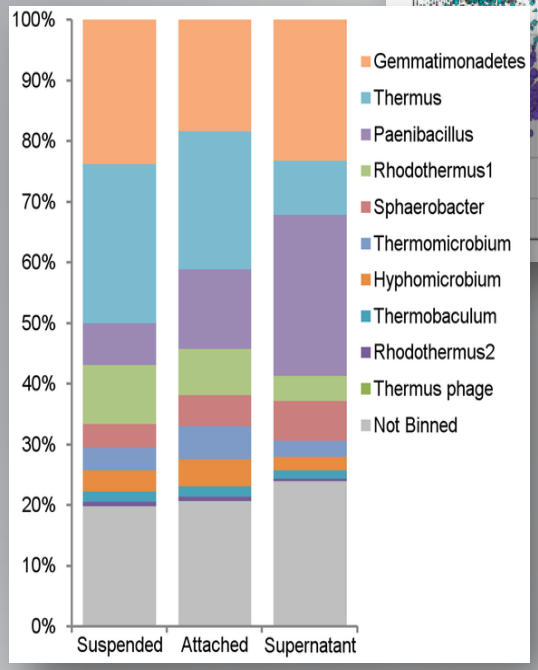
Pel et al., 2007. Nature Biotechnology 25, 221 - 231

10 year goal: Provide an understanding of how cells compartmentalize metabolic reactions and pathways to inform predictive models.

Microbes whose enzymes deconstruct switchgrass identified

JBEI/JGI/EMSL

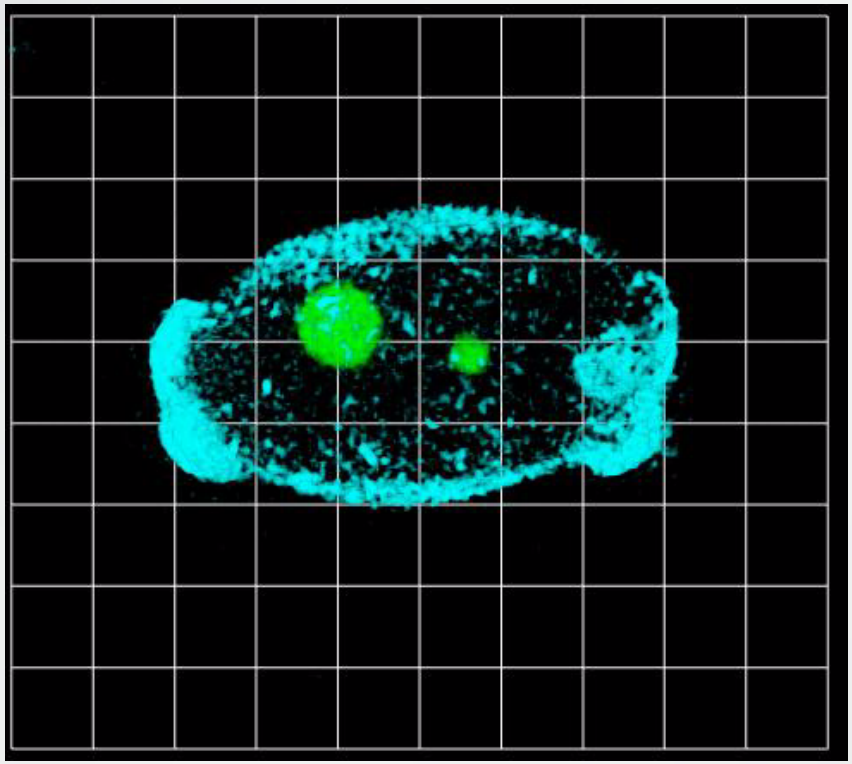




Institutions: *JBEI, LLNL, SNL, JGI, Leibniz Institute of Freshwater Ecology and Inland Fisheries, LANL, PNNL, EMSL, The University of Queensland, LBNL.*

Reference: *D'haeseleer et al. 2013 PLoS ONE 8(7):e68465.*

Yarrowia lipid production in time and space



Participants: *MIT, PNNL, UCLA*

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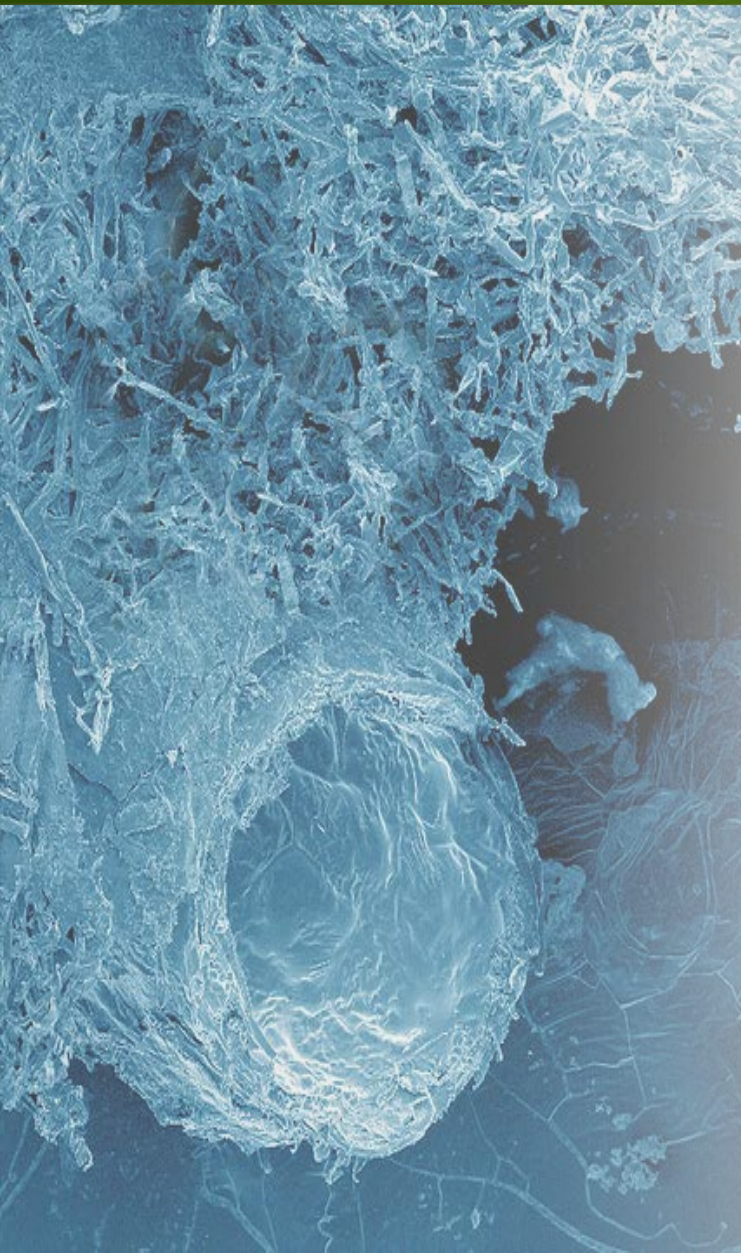
Terrestrial and Subsurface Ecosystems



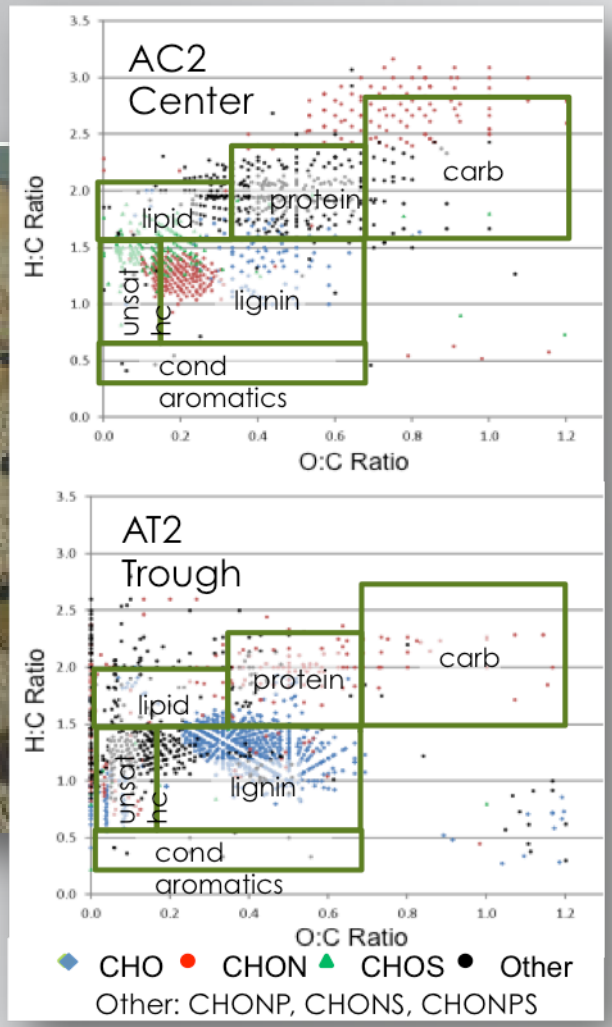
Our focus: Understanding nutrient, metabolite, and chemical signature flux at biogeochemical interfaces in heterogeneous environments across multiple scales.

Of special interest: Molecular to pore scale understanding of hydro-biogechemical elemental cycling.

Molecular to pore scale understanding of hydro-biogeochemical elemental cycling

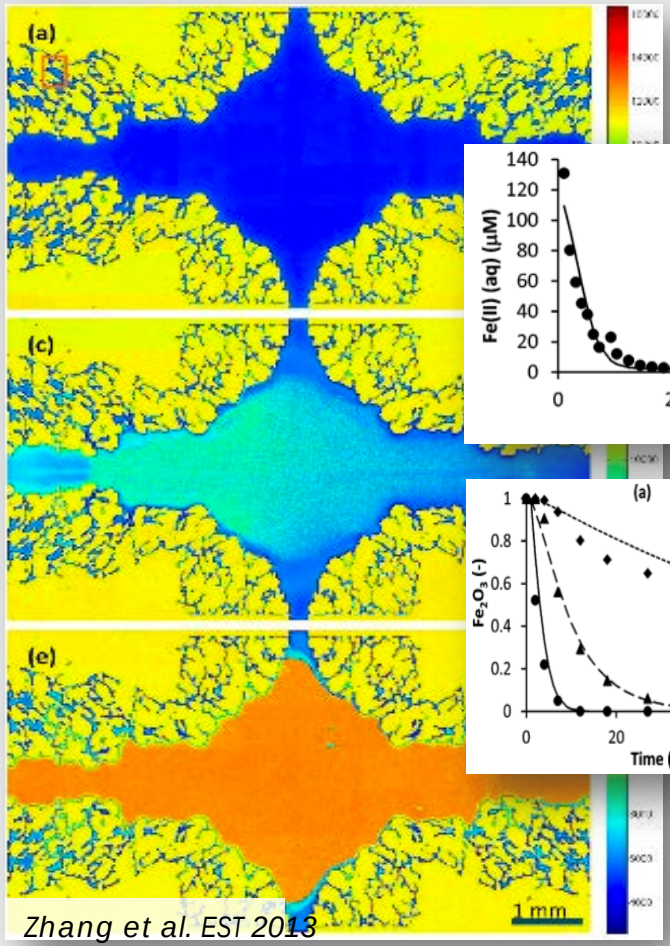
10-year Goal: Molecular-to pore-scale understanding of the coupled biogeochemical and elemental cycling processes that advance predictive understanding of the water cycle and ecosystem biogeochemistry feedbacks and inform the biogeochemistry components of the ESM.

NGEE Arctic pore water extracts



Participants: Baohua Gu, ORNL

Visualization and modelling of pore-scale microenvironments



Zhang et al. EST 2013

Participants: Zhang, Chevron EnvSciTech 2013

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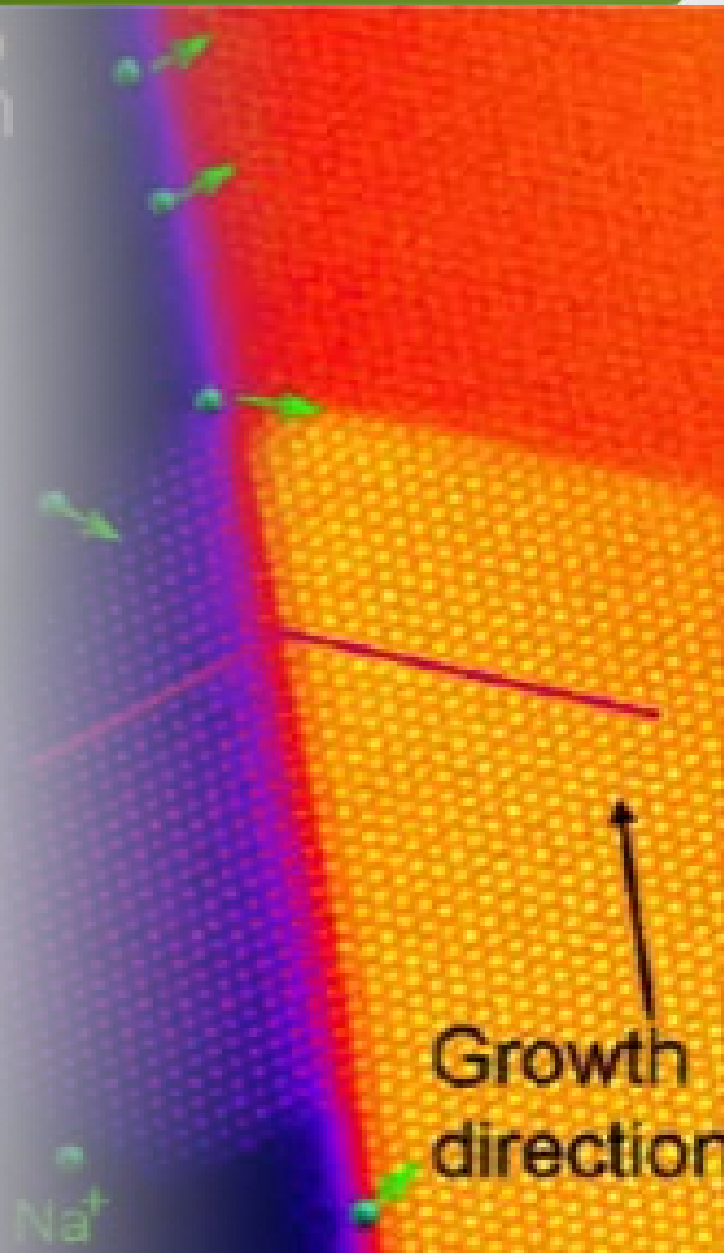
Energy Materials and Processes

Our focus: Understanding of the physical and chemical phenomena, with special attention to interfaces, needed to design new materials and systems for sustainable energy applications.

Of special interest: Solvent mediated interfacial chemistry.

Solvent mediated interfaces

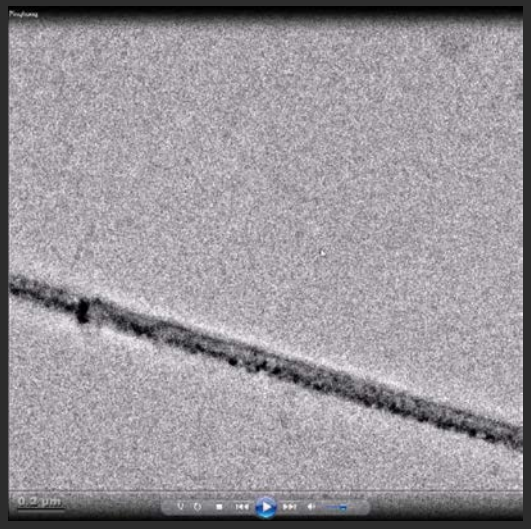
10-year Goal: Understanding processes at solvent mediated interfaces to predict the transformation mechanisms and physical and chemical properties needed to design advanced batteries and new catalysts.



EMSL researchers develop more realistic methods to study battery electrodes in action

Scientific Challenge

Microscopic observation of battery electrodes during cycling in liquid environments has been nearly impossible



Results

- EMSL, ORNL, and Northwestern University developed a microscopic view of battery electrodes while bathed in wet electrolytes, mimicking realistic conditions inside batteries and providing insights into how electrodes behave chemically.

Why It Matters

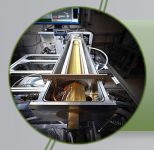
- Metal ions squeezing into the electrode's pores makes the electrodes swell, and repeated use can wear them down ultimately leading to battery failure. Understanding electrode function will enable the development on longer lasting batteries.

Computation and data visualization

Imaging and microscopy

Spectroscopy and diffraction

Synthesis and microfabrication



-Omics

Radiochemistry

1. **Evaluated** against key criteria: impact, uniqueness, operations
2. **Selected and assessed** with input from Advisory groups, users and stakeholders
3. **Emphasis** on operando and dynamic measurements

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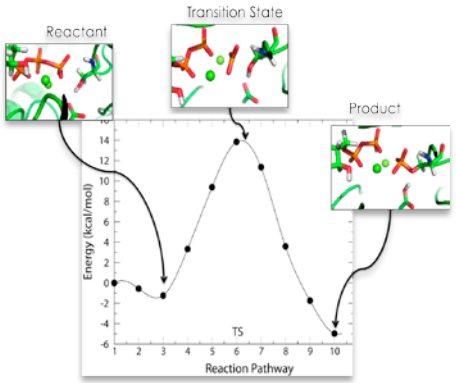
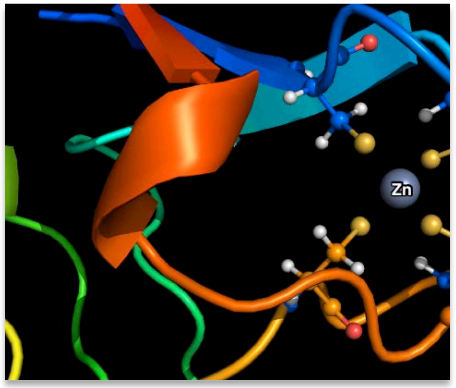
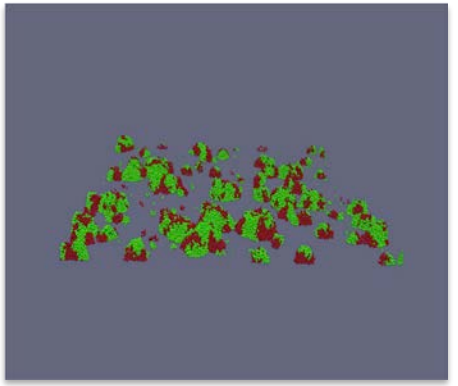
Computational and data visualization capabilities



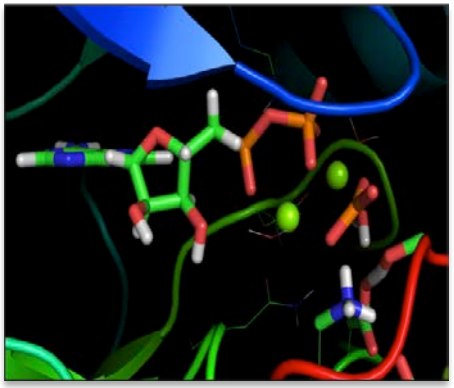
Free Energy calculations



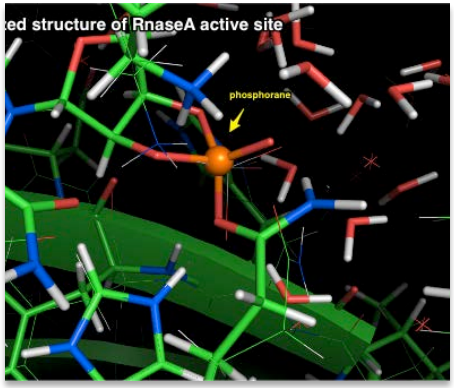
Properties



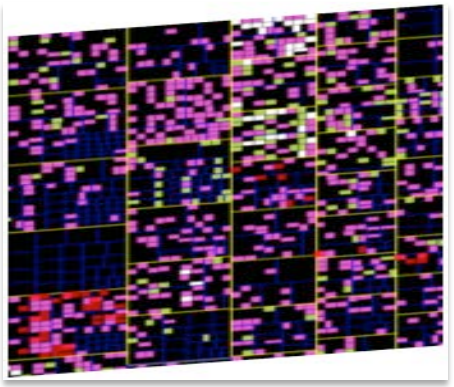
Modelling communities



Reaction pathways

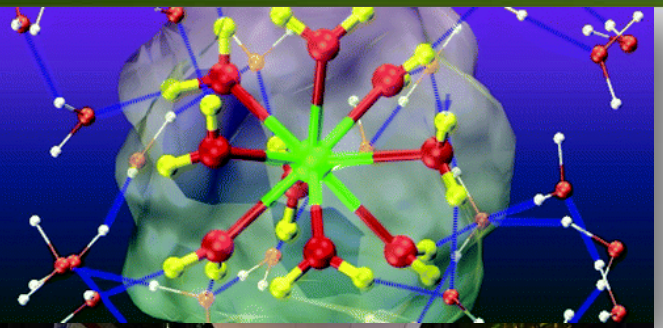


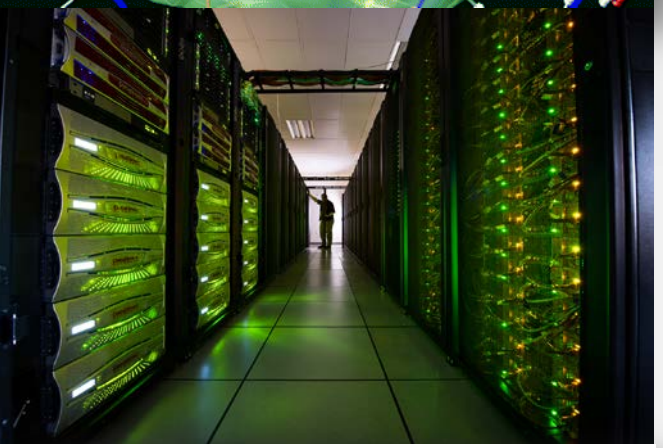
Structural characterization

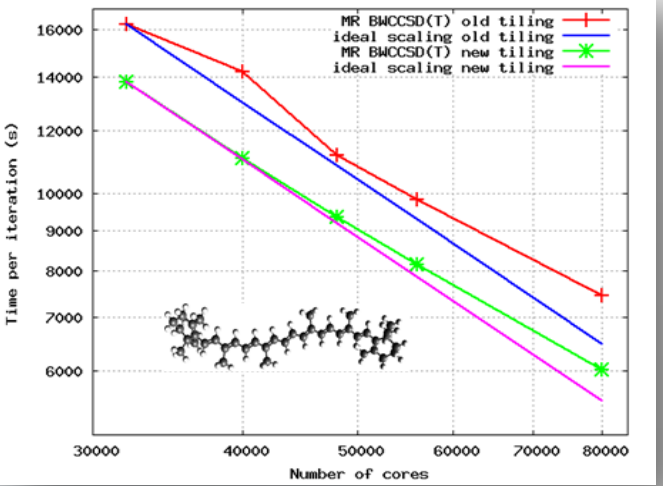


IMPROV+

Theory and High-Performance Computing

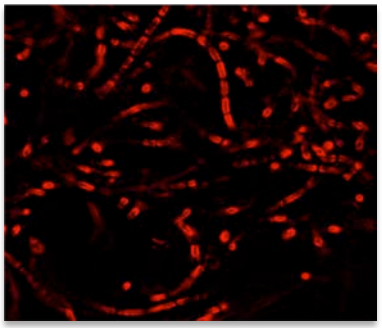




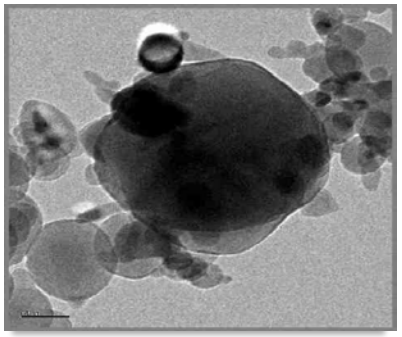


- HPC-Enabled Science
  - Accurate state-of-the-art algorithms for computational chemistry, spectroscopies (NMR, X-ray, UV/Vis), excited-state dynamics
- Future Directions
  - Predictive models increasing in scale from nano- to meso-scale systems relevant to larger-scale scientific problems (aerosol properties, soil aggregates, biocatalysis)
- Cascade: #13 on Top 500
  - Speeding up NWChem using heterogeneous computer architectures (Xeon Phi processors)

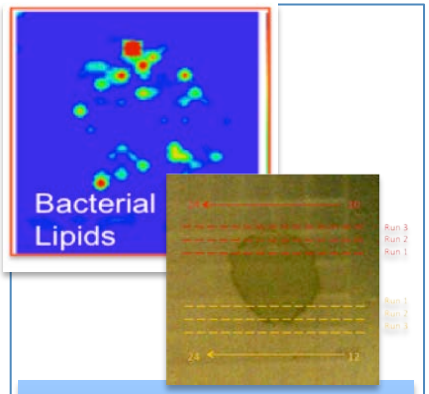
Imaging capabilities



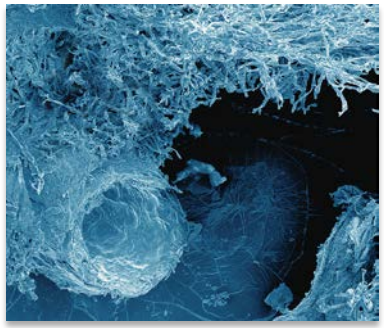
Structured illumination microscopy



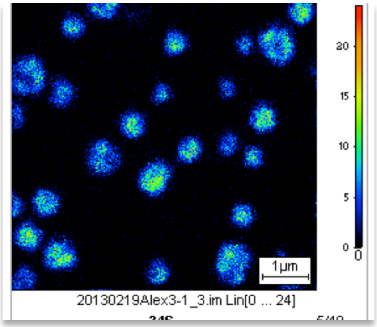
Transmission electron microscopy (static and dynamic)



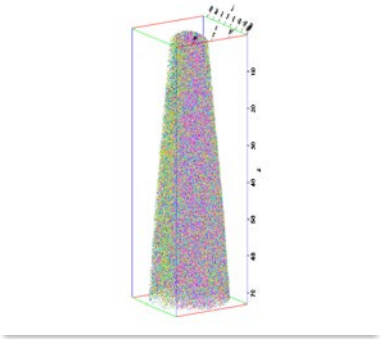
Mass microscope



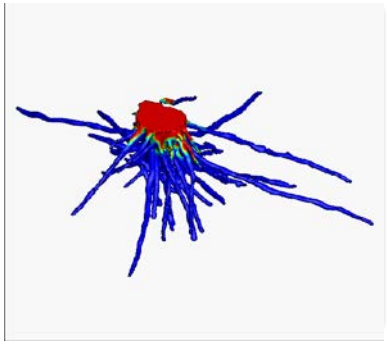
Scanning electron and Helium ion microscopy



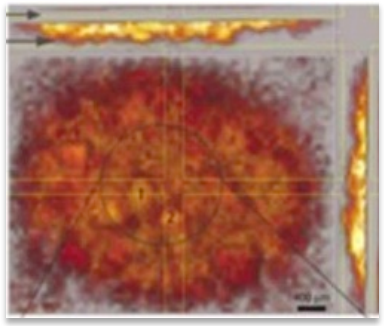
NanoSIMs



Atom probe

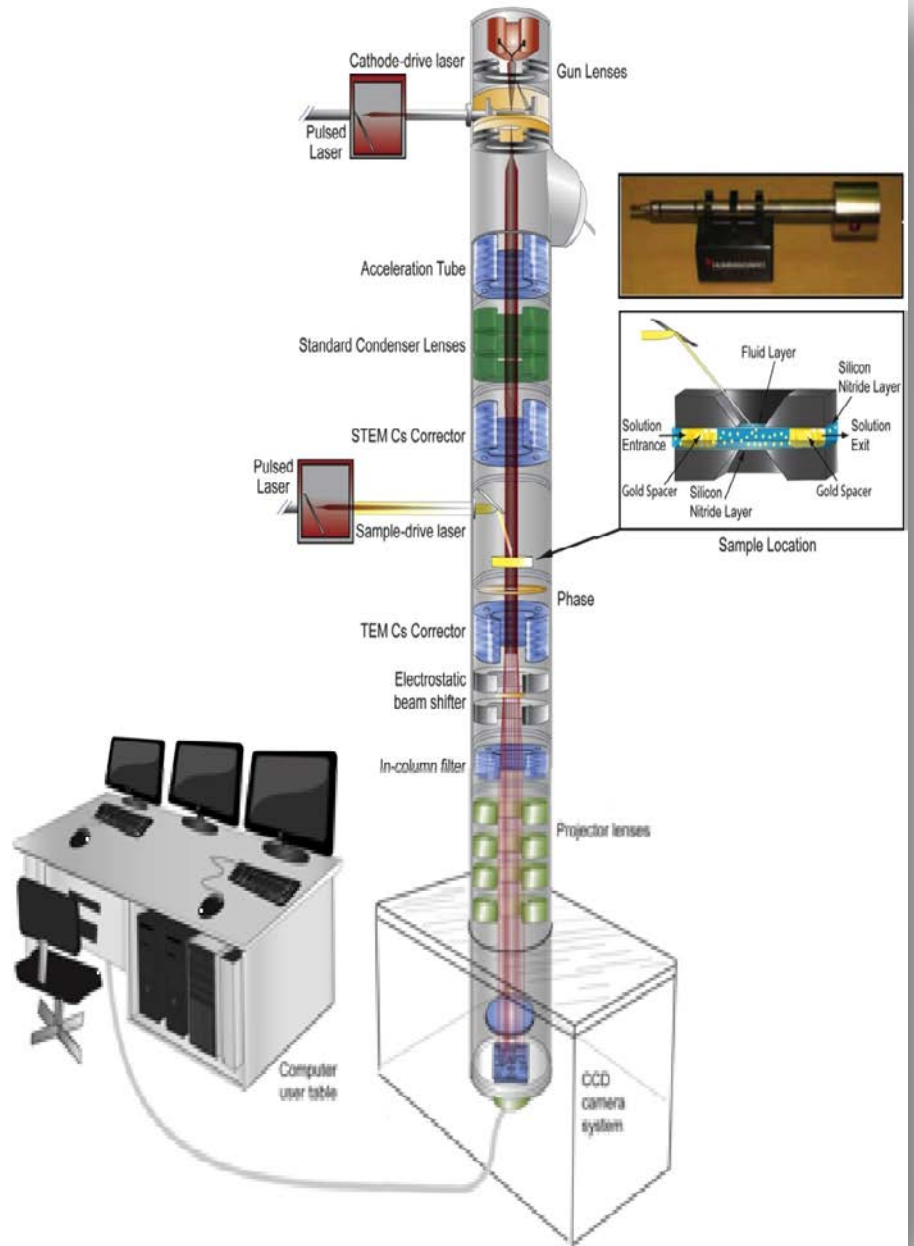


Tomography



Magnetic resonance imaging

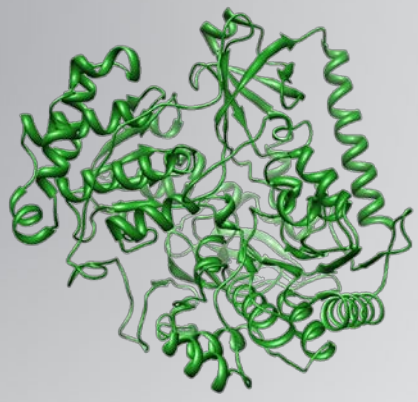
Dynamic TEM prime for probing dynamic systems



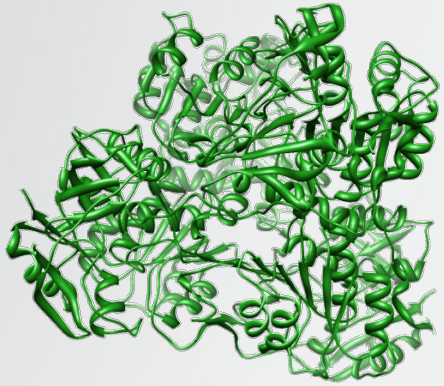
- Aberration correction
- Tunable
- Near-atomic spatial resolution down to 50 ns temporal resolution
- In-situ liquid compatibility

Imagine the possibility of uniting structure-based design with dynamic observations to enable the rational design of biosystems.

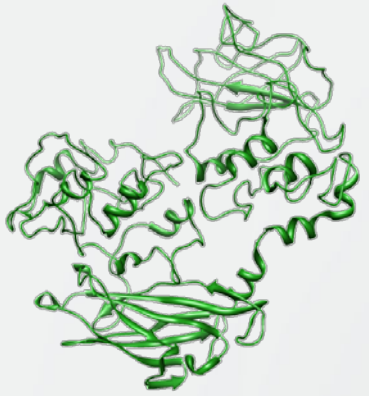
Requires a mechanistic understanding of how reactivity is related to structure AND temporally resolved molecular motions.



Formate Dehydrogenase



Alcohol Dehydrogenase



Decaheme Cytochrome

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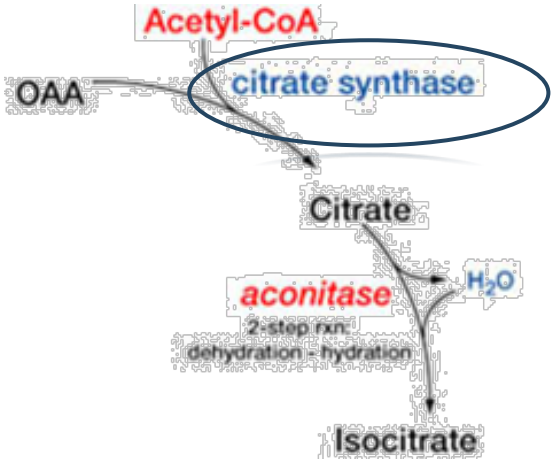
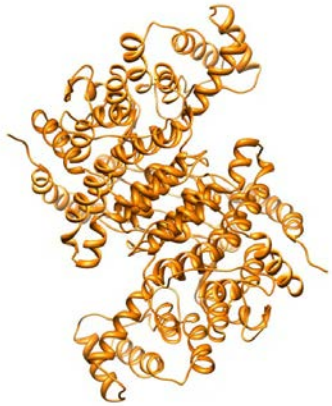
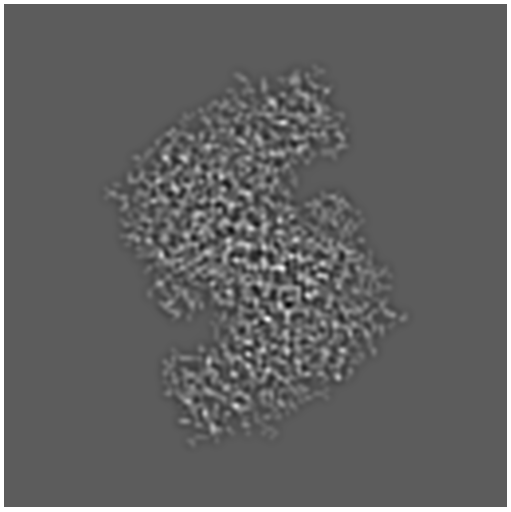
Dynamic TEM designed to visualize protein motions in real-time



Ribbon simulations morphing between known starting and ending structures of citrate synthase

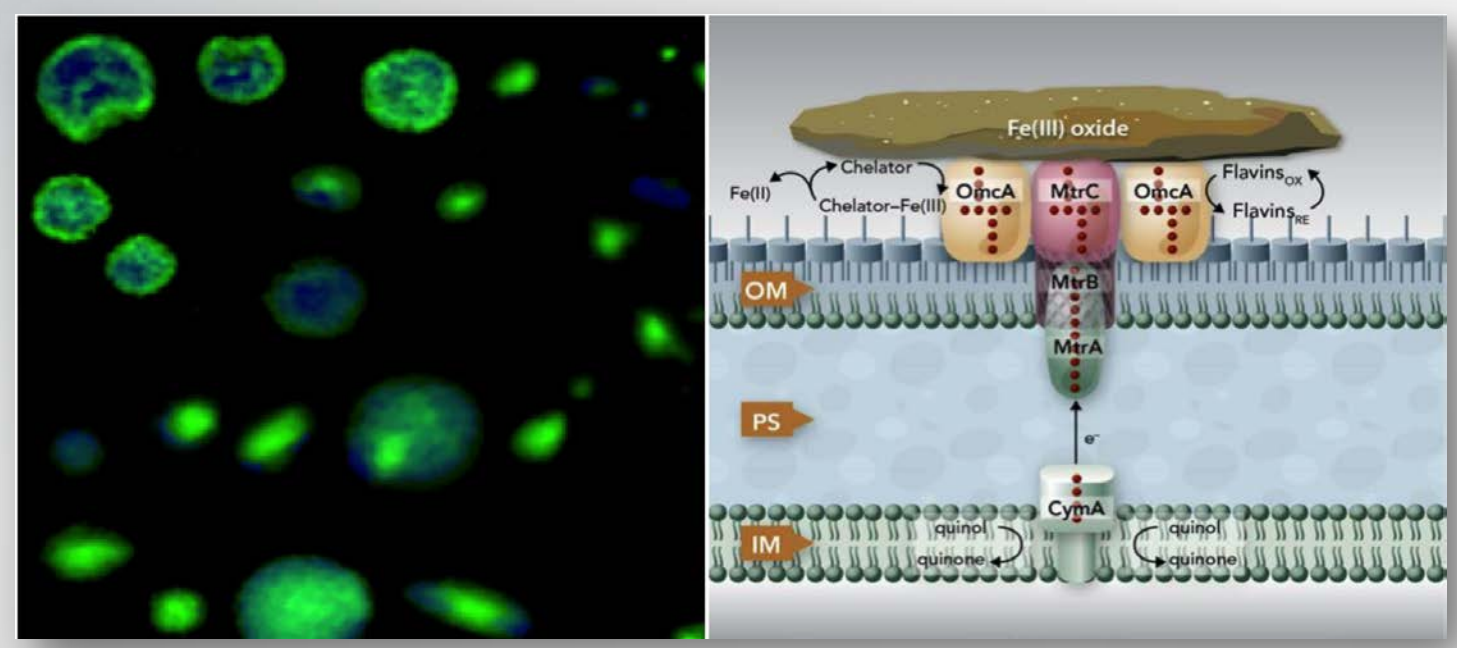


TEM Image morphing between known starting and ending structures of citrate synthase



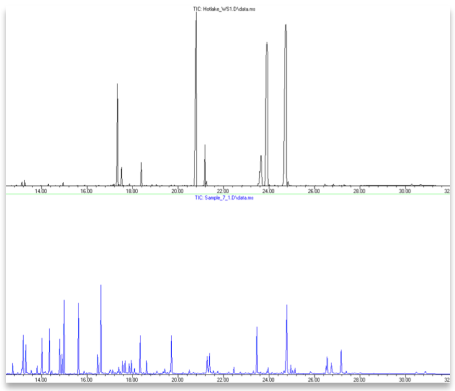
Visualizing the dynamics and motions of proteins in native environments could identify key amino acids for enhancing biodesign to control metabolism or engineer more efficient isozymes

Potential science challenges for DTEM

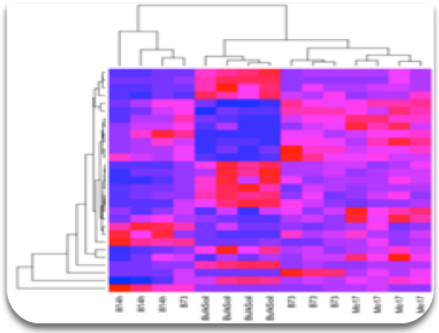


- Unravel how weak organic acids mixed with sea salt modify particle properties related to climate and effect balance of oxidants in the atmosphere
- Discover the structure and function of multi-heme cytochromes and their cognate complex partners that facilitate electron transfer

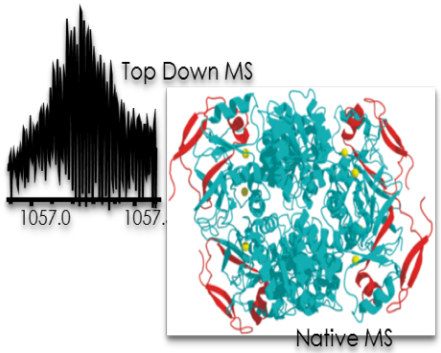
-Omic and molecular species characterization



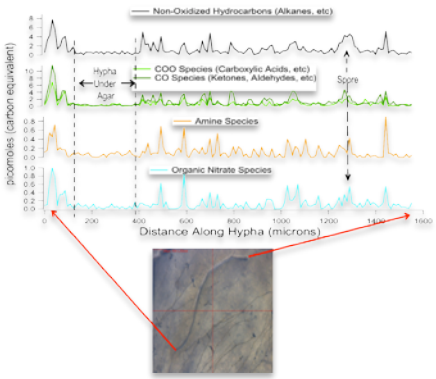
Metabolomics



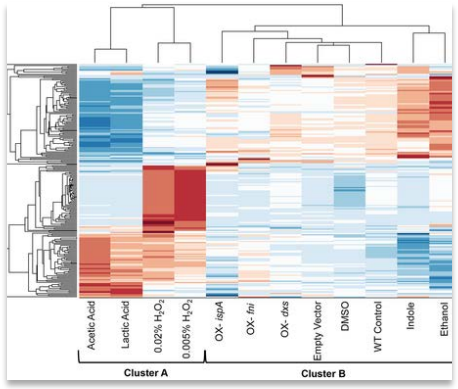
Bottom up proteomics



Top down proteomics

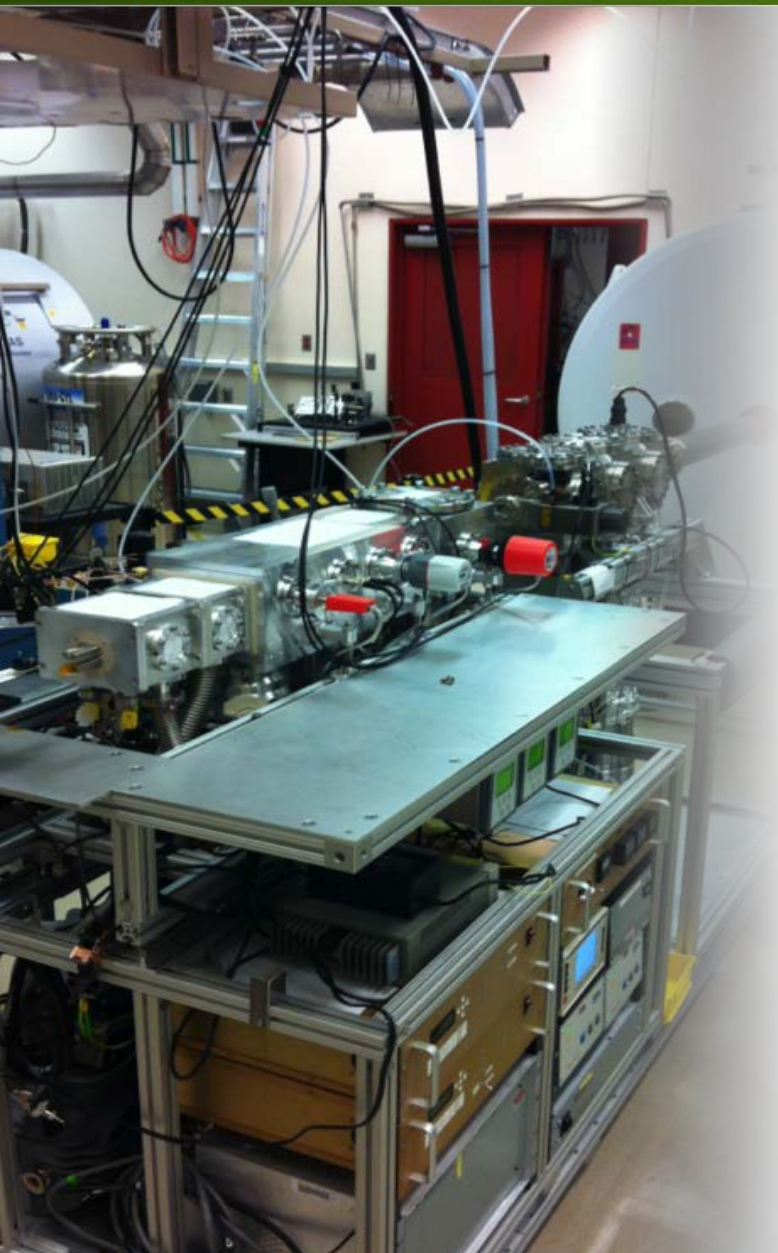


Molecular species



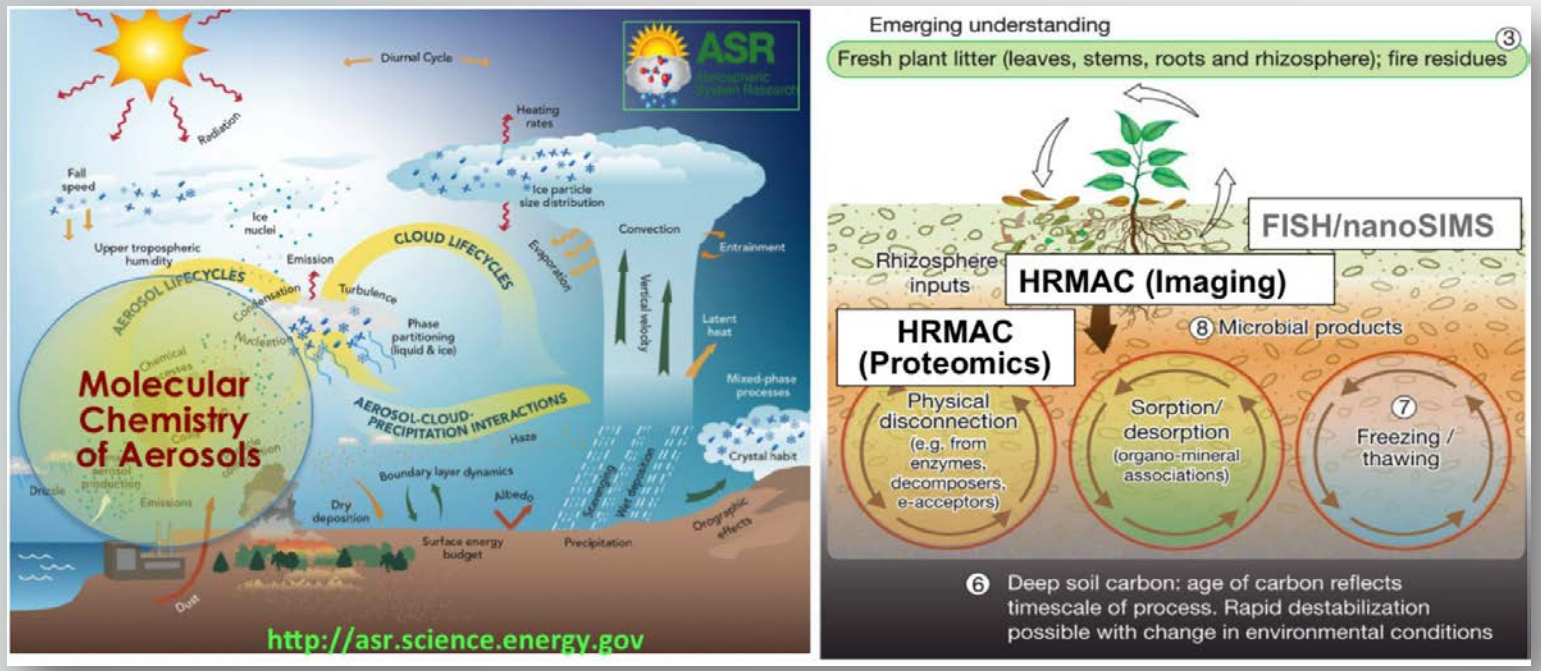
Transcriptomics

Scientific Drivers for HRMAC



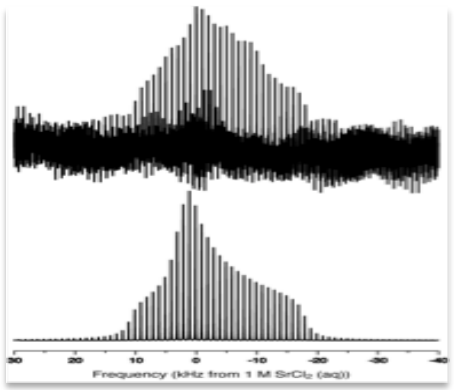
- Unraveling complex environmental and biological mixtures
- Linking genotype to phenotype to predict biosystem behavior
- Functional understanding of microbial metabolites
- Decoding the chemical language of bacteria, fungi and plants

Science challenges for HRMAC

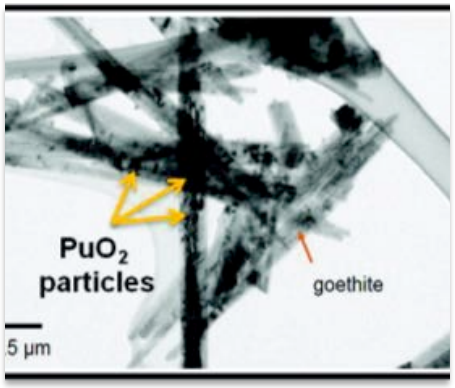


- Develop comprehensive molecular level profiles of aerosol composition and its variability and impacts
- Reveal molecular scale understanding of soil structure and heterogeneity thus linking processes with the biota

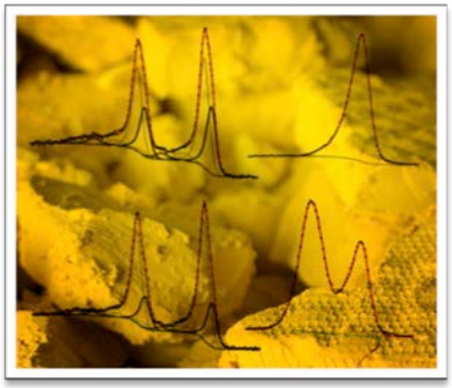
Radiochemical



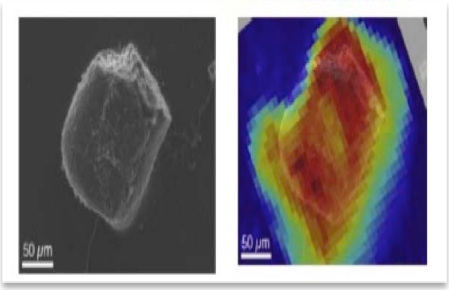
Magnetic resonance



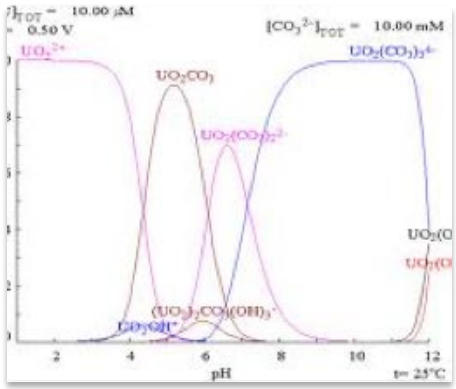
Microscopy



XPS

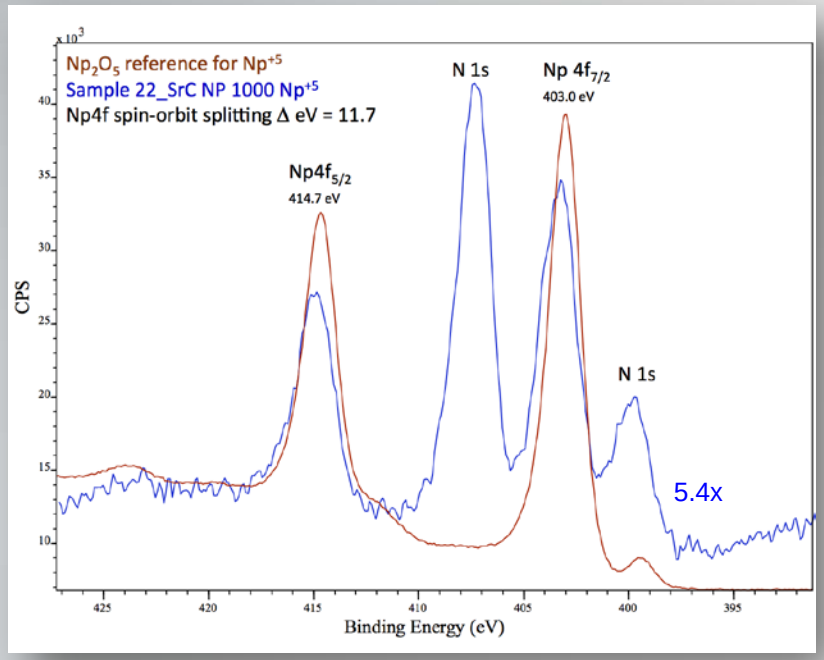


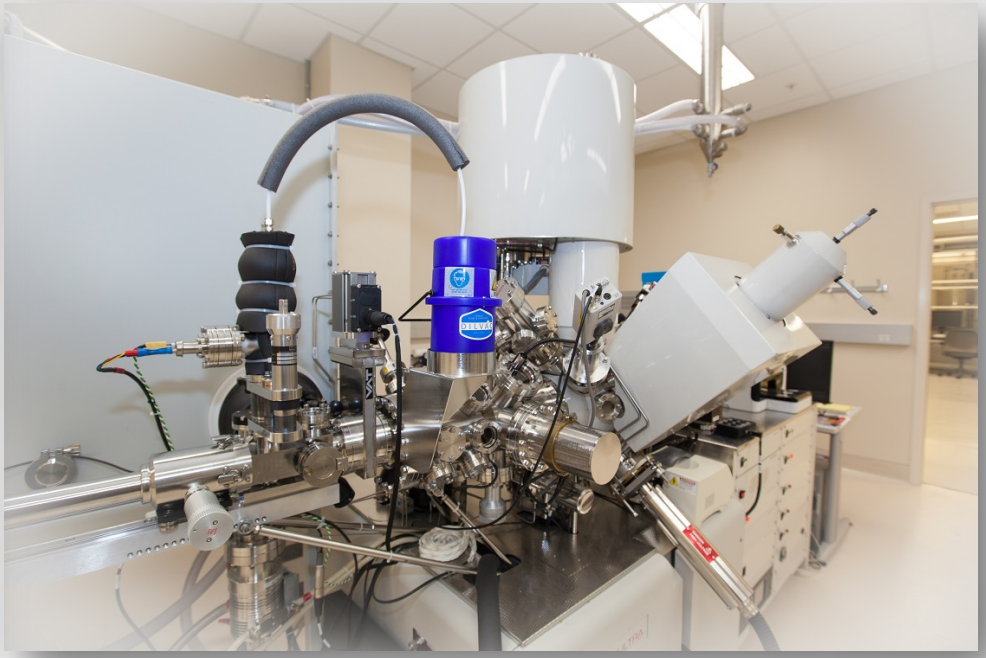
Electron microprobe

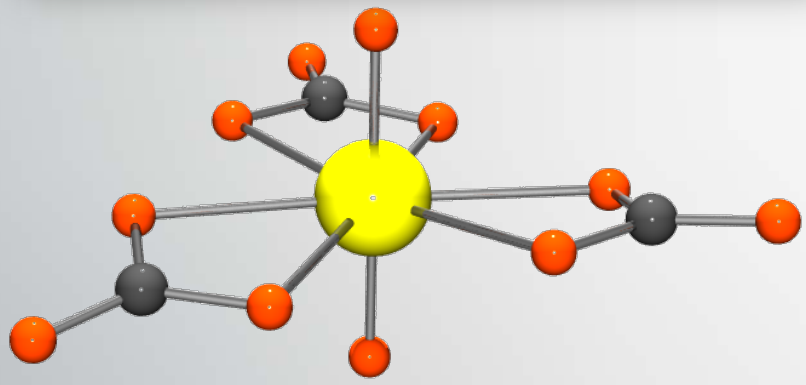


Analytical

NpO_2^+ Environmental Chemistry: Incorporation in low temperature secondary minerals



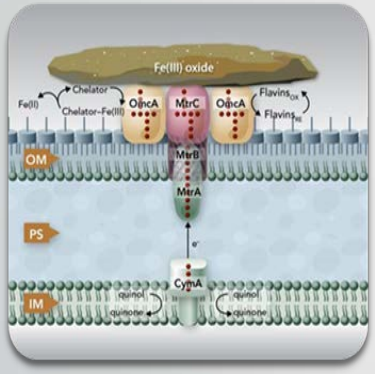


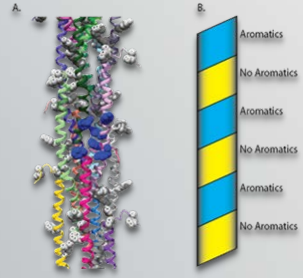


Users: Peter Burns (director) and Enrica Balboni, University of Notre Dame, Materials Science of Actinides EFRC

Understanding metabolism in space and time

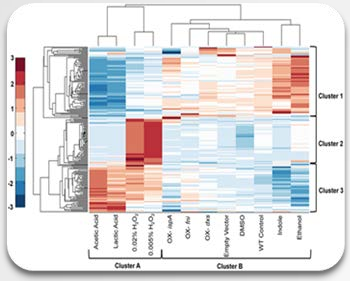
Observe protein complexes assemble and visualize conformational changes during the enzymatic process: DTEM

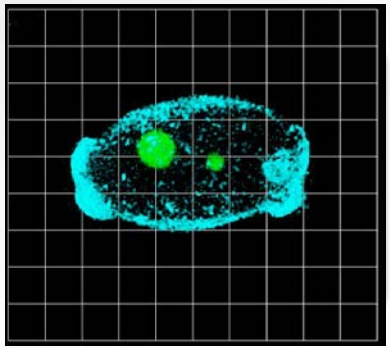




Protein structure elucidation: NMR

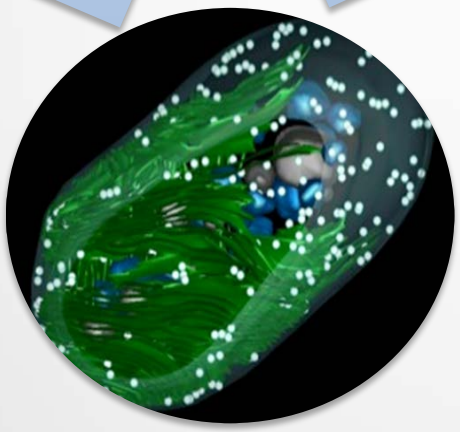
Decipher metabolic networks and enable genetic engineering approaches: integrated omics

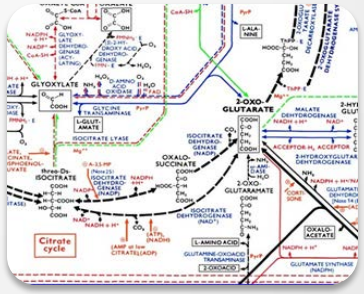




Visualization of biological compartments: SIM

Visualization of ultra-structures and whole cell reconstruction: TEM

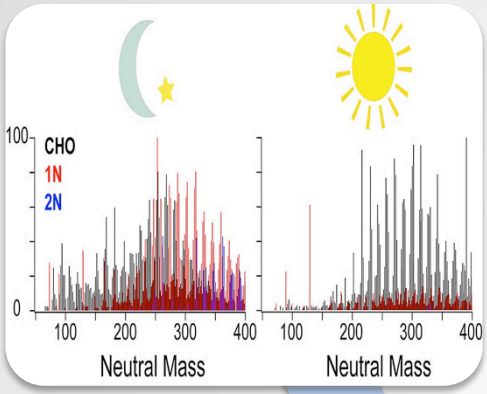




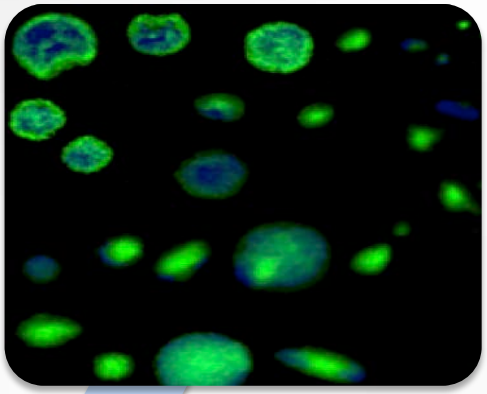
Model pathways: Modeling & simulation

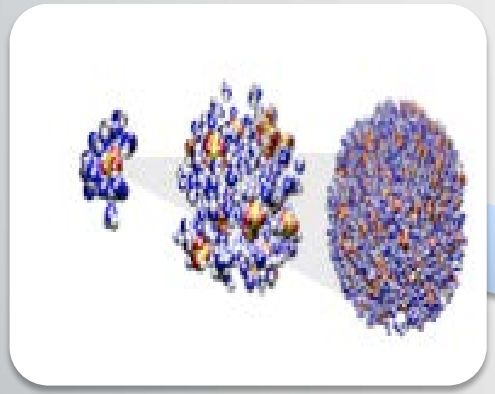
Understanding Dynamic Processes in Biogenic Organic Aerosols

Source identification - MS



Particle composition and morphology - SEM



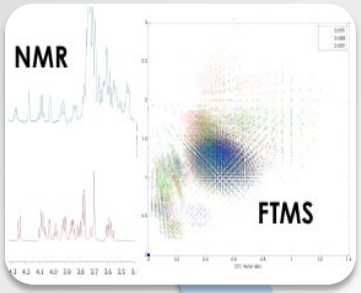


Optical properties; nucleation, photochemistry - computation

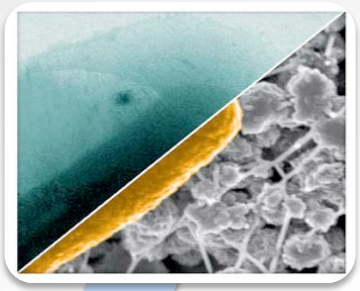
Field studies and *in situ* analysis

Understanding Soil Carbon Dynamics

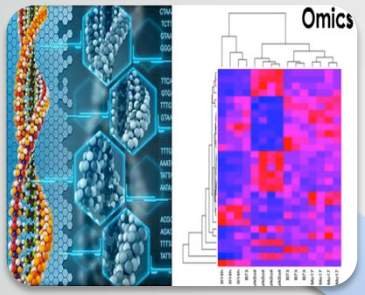
Organic matter characterization – NMR, MS



Geo and Biogeochemistry - Microscopy

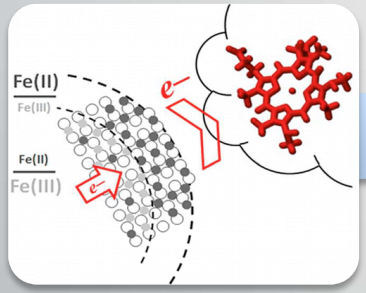


Microbial community characterization – MS, microscopy, JGI

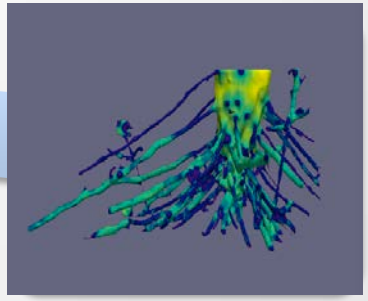


Hydrology and pore scale dynamics – Microfluidics and simulation

Electron transfer - computation



Root structure – X-ray computed tomography

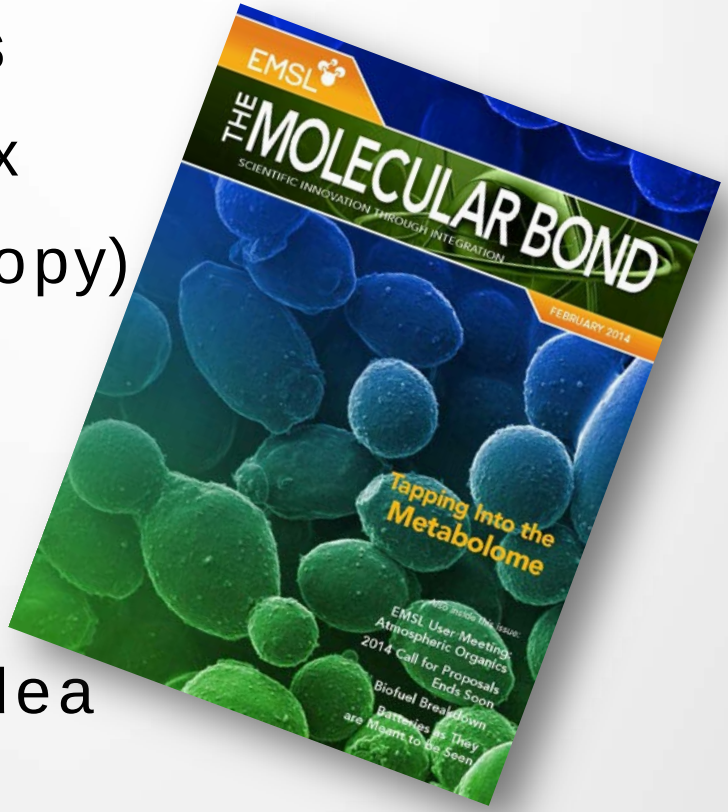


10^{-9} m

10^{-3} m

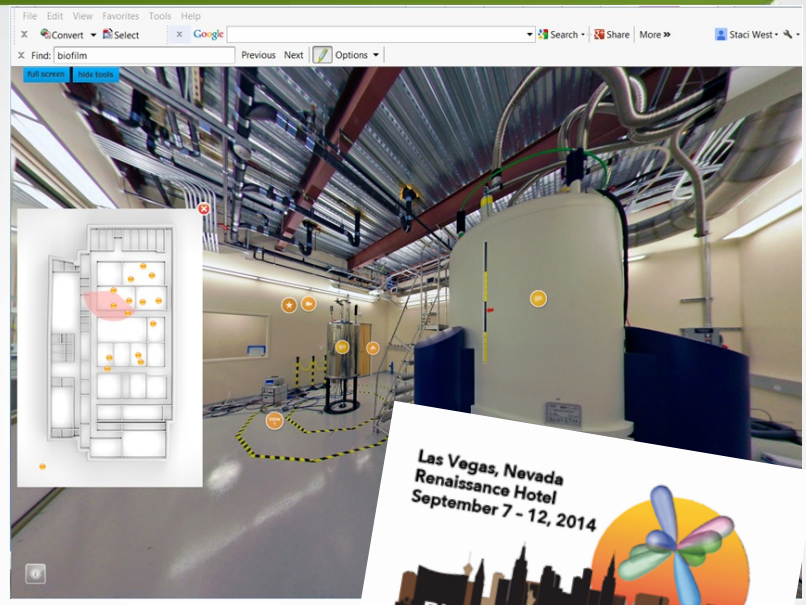
Outreach highlights EMSL expertise, science and opportunities to targeted audiences

- Focused User meetings
  - FY13: Plants, microbes and their Interactions
  - FY14: Science of Atmospheric Organics
- Features highlight new capabilities
  - CENews: Radiochemistry Annex
  - DOE web: Quiet wing (microscopy)
- NUFO Congressional event
- Molecular Bond
- Inviting BER-funded PIs to EMSL
- Developing "EMSL Open House" idea

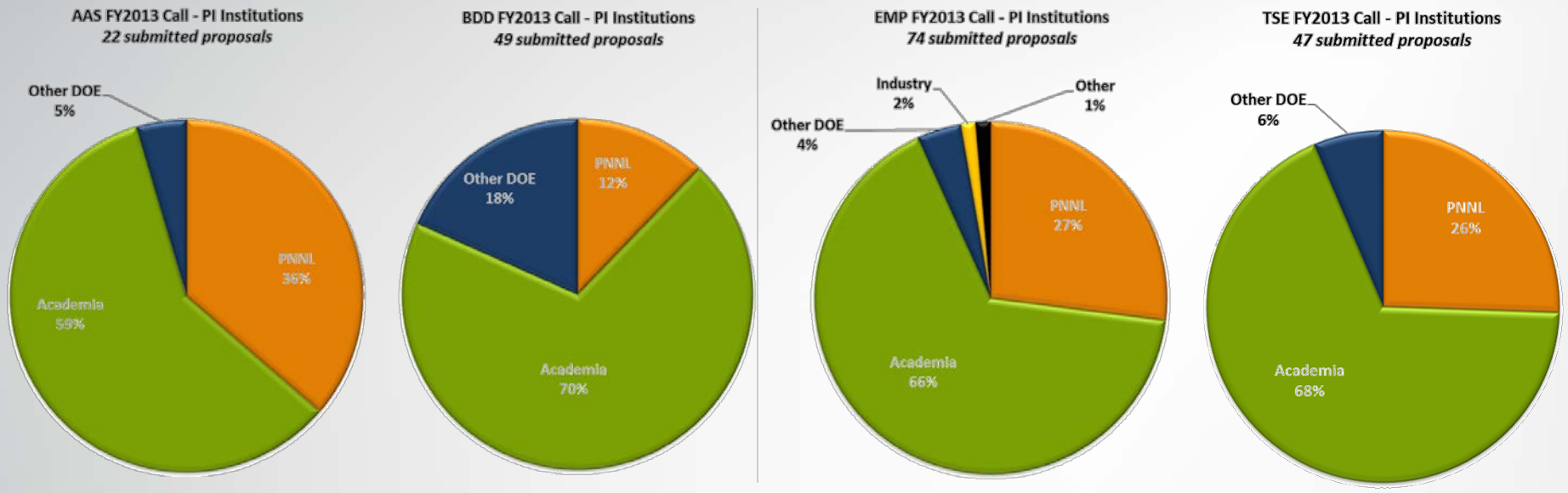


Reaching out to the radiochemistry community

- Developed virtual tour
- Invited to speak at Pu Futures meeting
- Part of Round Robin Test in Actinide Spectroscopy
- Meeting with EM program managers

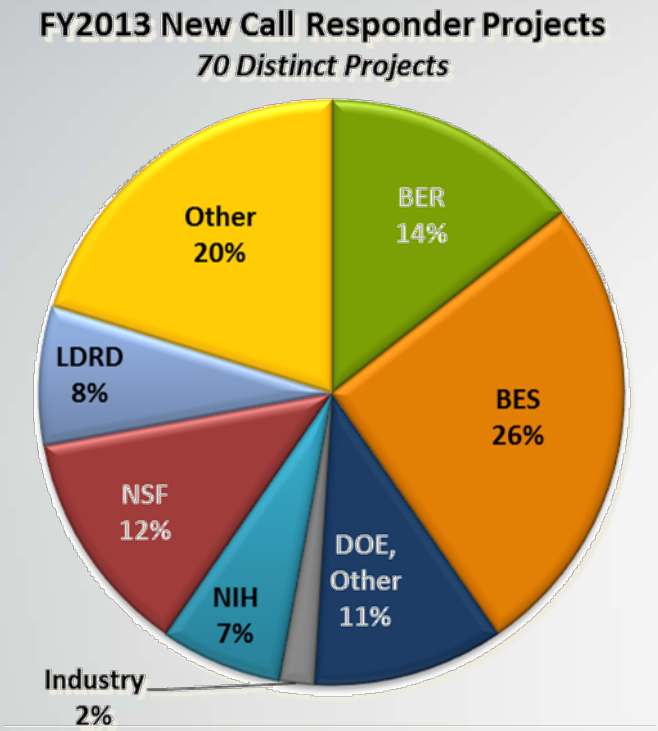


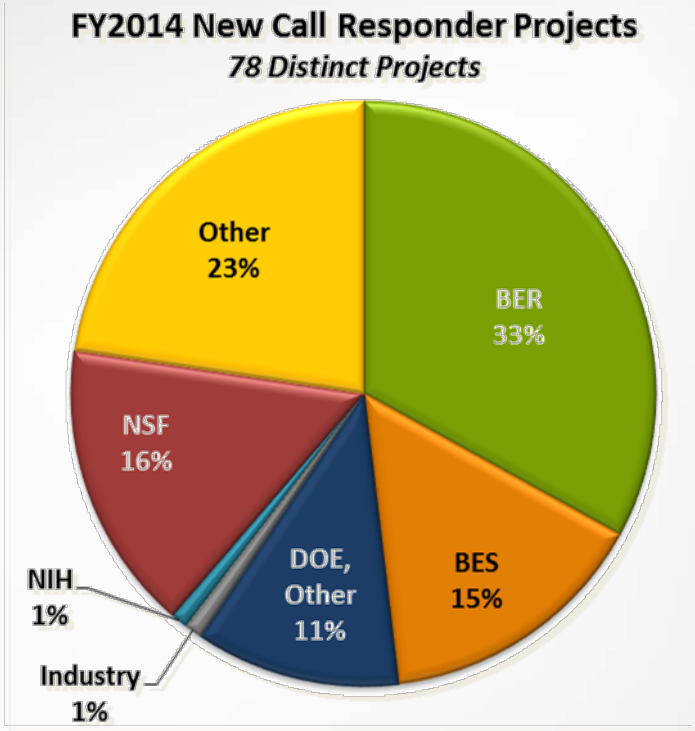
FY 13 Science Theme call was very successful in attracting external participants



- Over ½ of the proposal teams were external to PNNL
- Almost ¼ of the teams were new to EMSL

Science Theme call was very successful in attracting BER-funded participants





Doubled the percentage of new BER-funded projects accepted to the call since FY13

Advisory Committees help shape EMSL strategy and operations

- Science Advisory Committee
  - Len Spicer, Duke (Chair)
  - Mark A. Barteau, U. of Michigan
  - Gordon E. Brown, Jr., Stanford
  - **Michael Celia, Princeton**
  - Sue Clark, WSU
  - Ian Farnan, U. of Cambridge
  - Barbara J. Finlayson-Pitts, UCI
  - **Scot Martin, Harvard**
  - **Gerry McDermott, UCSF**
  - Julia Rice, IBM Almaden Research Center
  - James M. Tiedje, Michigan State University
  - **Soichi Wakatsuki, Stanford**
  - 2 TBDs

Next meeting: June 3-5

- User Executive Committee
  - Angela Wilson (Chair), UNT
  - Paul Tratnyek (VC), OHSU
  - **Simon R. Bare, UOP LLC**
  - David A. Dixon U. of Alabama
  - Mary Gilles, LBNL
  - Steven Hallam, UBC
  - John V. Hanna, U. of Warwick
  - **Matthias Hess, WSU**
  - Anne Johansen, CWU
  - **Daniel Knopf, Stony Brook**
  - Matthew McCluskey, WSU
  - Sergey Nizkorodov, UCI
  - **Jennifer Pett-Ridge, LLNL**
  - Roger Rousseau, PNNL
  - **Louis A. Sherman, Purdue**
  - **Blake A. Simmons, JBEI, SNL**
  - Charles Werth, UIUC

Next meeting: May 5

User opportunities

- Annual Science Theme call (closes 3/3/14)
- JGI-EMSL Collaborative Science call (closes 4/7/14)
  - Biogeochemistry
  - Carbon Cycling
  - Biofuels
- First Science
  - DTEM and HRMAC

On the horizon

- EMSL User meeting: May 6
- NUFO Annual Meeting: April 30-May 2
- Triennial Review: September 23-24

EMSL

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Questions?