

- **Bacterial ‘cell-cell talk’ in complex microbial communities: identifying diverse and novel quorum sensing signals in extreme environments**



ALAN WILLIAM DECHO

University of South Carolina

Microbes communicate using quorum sensing that occurs within/among microbial species to synchronize gene expression and provide adaptive responses to stress. Researchers will use EMSL’s lipidomic and metabolic capabilities to identify and characterize new putative signals for quorum sensing systems and determine how relative concentrations change with environmental stress.

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- **Wildfire impacts on organic matter bioavailability and river corridor biogeochemistry**
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ALLISON N MYERS-PIGG

Pacific Northwest National Laboratory

Researchers will examine how the chemistry of pyrogenic organic matter changes with various burn severities by manipulating burn conditions and feedstocks, which will allow for increased predictive understanding of the impact fires have on river corridor hydro-biogeochemistry..

• Waterborne plastics environmental weathering leachates



BENJAMIN DUDLEY MAURER

National Renewable Energy Laboratory

This work will leverage planned field measurements, with EMSL characterizing leachates—such as environmental weathering products, additives, and persistent organic pollutants—contained in collected water samples from five U.S. rivers. The findings will further improve understanding and valuations of the environmental, social, and health costs of aquatic plastic pollution.

- **Comparative systems analysis of bioenergy grass internode development for biofuel production in marginal environments**
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ANDREI SMERTENKO, KAREN SANGUINET, & LAURA BARTLEY

Washington State University



This project will enable the development of a predictive model for conserved vascular bundle developmental circuits in internodes and will aid the engineering of bioenergy grass varieties with increased yields and improved composition in marginal environments.

- **Analysis of biogeochemical nutrient delivery to the Amazon and Atlantic Ocean from transported smoke and dust**



CASSANDRA JAYNE GASTON

University of Miami

Researchers will analyze samples of atmospheric particles from sites in the Amazon Basin and in Barbados that have documented dust transport for more than 50 years. This will improve understanding of how aerosols fertilize ecosystems and affect the global carbon cycle through the sequestration of atmospheric carbon dioxide.

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- The effect of acyclic terpene emissions on secondary organic aerosol properties
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CELIA LOUISE BRAUN FAIOLA

University of California, Irvine

This research will provide the first comprehensive investigation of secondary organic aerosol chemistry from acyclic terpene oxidation and will be the first to evaluate the effects of plant stress volatile emissions using a regional chemical transport model.

- Mechanisms of soil organic matter stabilization across a phosphorus and land use gradient in carbonate lithologies
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CHRISTOPHER BRIAN SHEPARD

University of Kentucky

Researchers will use EMSL resources to establish the importance of phosphorus in supporting soil organic matter stabilization on soil mineral surfaces relative to other biocritical nutrients as well as the extent to which the relationship between the belowground carbon and phosphorus cycles is altered by human land use.

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- **High-resolution spatiotemporal modeling of root-associated microbial communities**
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DANIEL SEGRE

Boston University

This project aims to implement high-resolution simulations of synthetic microbial ecosystems around the roots of plants. Researchers will run simulations of rhizosphere communities to obtain unprecedented insight and testable predictions, paving the way for a new generation of multiscale models of plant–microbe–environment interactions and dynamics.

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- **Micro to macro – molecular and spatial controls on microbial function**
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DARIAN SMERCINA

Pacific Northwest National Laboratory

Establishing a clear and predictable link between the structure and function of soil microbial communities and ecosystem processes remains one of the greatest challenges in soil ecology.

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- **Reliable computational studies of the role of metal dications in organic complexation and mineral formation and the formation of atmospheric acid gases**
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DAVID ADAMS DIXON

University of Alabama

Researchers will use computational chemistry approaches on EMSL's advanced computers to quantitatively study the interactions of metal dications with organic materials, which are important for carbon dioxide capture and sequestration, biomineralization, and carbon cycling. This will enable a new understanding of the controlling physical phenomena at different spatial scales.

- # Understanding simultaneous lignin depolymerization and catabolism in white-rot fungi
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DAVINIA SALVACHUA RODRIGUEZ

National Renewable Energy Laboratory

White-rot fungi (WRF) are responsible for a substantial amount of carbon turnover on Earth. Researchers will use EMSL's advanced multi-omics capabilities to better understand this regulation and continue elucidating extracellular and intracellular lignin catabolic pathways in WRF. This information will improve understanding about global carbon cycling in soil ecosystems.

- Identifying particulate organic matter in X-ray computed tomography images of soil aggregates with a deep learning approach



DEVIN ANDREW RIPPNER

United States Department of Agriculture - Agricultural Research Service

Researchers will use maps of particulate organic matter generated by FTIR microscopy, SEM-EDX, and corresponding X-ray CT to train a network to rapidly identify matter and minerals in images of soil aggregates.

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- The role of Fe(oxyhydr)oxides in regulating the biogeochemical cycling of the essential micronutrients zinc and copper
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EUGENE SAUL ILTON

Pacific Northwest National Laboratory

This project will determine the precise way that Fe (oxyhydr)oxides incorporate the essential micronutrients Zn and Cu, increasing our understanding of factors that influence their bioavailability, particularly in highly weathered terrains.

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- **Understanding the genetic and structural bases of hornworts' carbon-concentrating mechanism**
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FAY-WEI LI

Boyce Thompson Institute for Plant Research

Researchers will use a combination of RNA-sequence, proteomics, and fluorescent and cryo-TEM imaging to start unraveling the genetic and structural basis of carbon-concentrating mechanisms in hornworts. The results of this research will likely open a new and unique window toward enhancing photosynthesis.

• Functional genomics of the root vascular system



GARY STACEY

University of Missouri - Columbia

Nitrogen (N) management will be a critical feature for the production of bioenergy crops, which are likely to be grown in sub-optimal soils low in N content. Data will inform future research to improve N use efficiency while yielding new information to understand vascular tissue function in plants.

- Investigating oiliness: systems comparison of photoautotrophic and heterotrophic lipid production in *auxenochlorella protothecoides*



JEFFREY LEO MOSELEY

University of California, Berkeley

This project will develop a systems-level understanding of the transition from growth to storage lipid biosynthesis in *A. protothecoides*. EMSL's mass spectrometry and chromatography expertise and capabilities will be employed to analyze proteomic and metabolomic changes associated with the transition, triggered by nitrogen limitation.

- **A colloid is born: understanding iron-rich colloid genesis and transformation for improved watershed biogeochemical models**



JOHN REEDER BARGAR

Stanford Linear Accelerator Center

Researchers will explore the identity of colloids using S/TEM, XPS, and Mössbauer. Associated organic molecules will be analyzed using FT-ICR-MS. Information will be combined with in-house synchrotron-based X-ray spectroscopy to advance process-level understanding of colloid dynamics and bring us closer to our goal of proper representation in biogeochemical predictive models.

- **Influence of adsorbed organic acids on soil mineral wettability**



JOHN STEVEN LORING

Pacific Northwest National Laboratory

This work uses an integrated experimental and computational approach to investigate how the fundamental process of water adsorption on soil minerals is influenced by adsorbed organic acids at humidities below water saturation. The research will provide fundamental insights relevant to organic nutrient bioavailability in soils and global carbon cycling.

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- Incorporating hydrologic perturbation and microbial processes into carbon budgets from coastal wetland soils
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KELLY CATHERINE WRIGHTON

Colorado State University

Wrighton Lab is working to understand the factors that control methane production in coastal wetlands and their responses to these expected hydrological perturbations in the future to better predict methane release from natural systems during a changing climate.

- **Understanding mechanisms coupling the fates of iron oxides, organic matter, and micronutrient metals at redox hot spots**
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KEVIN MICHAEL ROSSO

Pacific Northwest National Laboratory

At redox hotspots, sorbed metals can be released by the interaction of ferrihydrite with Fe(II) by mechanisms that remain poorly understood. This project tackles this knowledge gap by focusing on the role of Fe(II)/Fe(III) electron transfer and its impacts on the bioavailability of sorbed metals.

- **Advancing micromodel and imaging capability to detect hotspots in the hyporheic zone**
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KEVIN ROBERT ROCHE

Boise State University

We will develop micromodels representing oxygen-saturated hyporheic sediments. We will use these micromodels to track the evolution of oxygen-depleted microzones resulting from feedbacks between biofilm growth and fluid flow. This capability will allow us to identify the biophysical processes and scales controlling reaction heterogeneity within the hyporheic zone.

- **Probing the Martian atmosphere and hydrosphere using micro- and nano-scale analyses**



KIMBERLY T TAIT-SENA

Royal Ontario Museum

This project aims to study hydrous Martian phosphate minerals in melt inclusions and to determine how sulfur isotopes have been disturbed within Martian sulfide minerals. This will allow for a more accurate prediction of phosphorous and water availability for life on Mars and the evolution of the Martian atmosphere.

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- The origin, occurrence, and distribution of water and volatiles in nominally anhydrous minerals
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MAHESH ANAND

The Open University

Researchers will utilize lunar samples to produce a wide array of volatile data, facilitating more accurate modeling of the origin and evolution of water in the inner solar system. This challenging analytical approach hinges on the correlation of structure and chemistry from atoms to planets.

- Investigation of organic matter interactions at geologically relevant mineral interfaces and metal cations
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NARASIMHAN LOGANATHAN

Michigan State University

The project will use classical and enhanced molecular dynamics simulation methods to determine the complexation behavior of organics at the different pores of geologically relevant clay minerals and will provide fundamental insights into interactions that dictate complexation mechanisms in the presence of naturally prevalent cations.

- Manipulating monocot (grass) lignin-forming dirigent protein complexes for optimal bioenergy/bioproducts



NORMAN G. LEWIS

Washington State University

The project will establish the biochemical basis for why grass lignocellulosic tissues are significantly less recalcitrant to biodegradation than their woody dicot counterparts. We will focus on a bio-feedstock, *Brachypodium distachyon*, to delineate the biochemical basis for the reduced lignocellulosic recalcitrance.

- A cross-scale modeling framework of organic matter biochemistry in river corridor system: scaling biogeochemical reaction kinetics from molecular to reach scales



PEIYUAN GAO

Pacific Northwest National Laboratory

This project will develop a machine-learning-informed multiscale modeling framework across the molecular, cell, and reach scales. The framework will be used to investigate the cycling of organic matter and its decomposition products between surface water and soil.

● Chemical imaging of particles from TRACER field study



RAJAN KUMAR CHAKRABARTY

Washington University in St. Louis

This project will provide a physico-chemical description of individual atmospheric particles collected to conduct systematic studies of composition and physical properties of airborne particles. The chemical imaging measurements will provide critical feedback for further development and evaluation of particle-resolved atmospheric models.

- Investigating fog processing of aerosol in amazonia and their climatic impacts



RICARDO HH GODOI

Federal University of Parana

This study aims to understand the chemical composition, morphology, and hygroscopicity of fog and cloud biological constituents and how they can affect the fog and cloud formation process. Researchers will use EMSL's high-resolution mass spectrometry platform to provide the molecular composition of bulk organic aerosol particles.

- **Contaminant immobilization through heterogeneous carbonate growth at mineral/water and mineral/microbe interfaces**



SEBASTIEN N KERISIT

Pacific Northwest National Laboratory

This research will investigate the effects of substrate-coating chemical interactions on the incorporation of metal contaminants in carbonate coatings and any enhancement in metal contaminant incorporation afforded by the formation of an amorphous calcium carbonate intermediate during microbially induced calcite precipitation.

- **CO₂ activation and conversion by the CODH/ACS enzymatic complex**



SIMONE RAUGEI

Pacific Northwest National Laboratory

This project will computationally characterize the mechanism of the carbon monoxide dehydrogenase and acetyl-CoA synthase complex, two enzymes that are the focus of intense biotechnological research because of their relevance to the “water–gas shift” and Monsanto industrial processes. Researchers will elucidate key enzymatic functionalities to drive the design of improved catalysts.

- **Dinitrogen activation and electron and proton delivery in the nitrogenase complex**



SIMONE RAUGEI

Pacific Northwest National Laboratory

Nitrogenases are key to the biological nitrogen cycle, providing the bioavailable nitrogen nutrient that supports more than half the human population. Researchers will use EMSL supercomputing resources to tackle the mechanism of electron and proton delivery to dinitrogen to yield ammonia in the Mo-dependent nitrogenase biological nitrogen fixation.

- **Role of Ca in organic matter preservation**



SHARON ELIZABETH BONE

Stanford Linear Accelerator Center

Calcium can play a major role in the preservation of carbon in the subsurface. Our work provides a foundational understanding of calcium organic matter complexation, which is necessary to develop thermodynamic and kinetic models of calcium complexation in the subsurface.

- **Biogeochemical consequences of microbial trait tradeoffs under drought, wildfire, and nitrogen addition**
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STEVEN DAVID ALLISON, BRIANNA K FINLEY, & EOIN BRODIE

University of California, Irvine & Lawrence Berkeley National Laboratory

This project will test a new trait-based theory of microbial metabolism that connects fire, drought, and nitrogen impacts with biogeochemistry at genome through community scales. The research will provide the missing link between genomic data and microbial metabolism by combining sequencing techniques with high-resolution metabolomics on soil microbiomes.

- **Understand how fungi cell wall responds to hypersaline environment**
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TUO WANG

Louisiana State University

This project aims to understand how fungi reconstruct their cell walls in hypersaline environments. Using EMSL's resources, researchers will characterize construction and composition to reveal the supramolecular architecture of microbial cell walls.

- Connecting the physicochemical properties with ice nucleation properties of secondary organic aerosols formed from multiphase chemical processes



YUE ZHANG

Texas A&M University

This project will provide new insights on how secondary organic aerosols generated from the multiphase reaction pathways will affect aerosol physiochemical properties and aerosol–cloud interactions. The outcome will be useful for improving current models in predicting aerosol transformation and future climate.