



User facility capabilities to accelerate impact in biomass

A presentation at Biomass 2010

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March 31, 2010



www.emsl.pnl.gov


Pacific Northwest
NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965



Mission

... to provide *integrated experimental and computational resources* for *discovery and technological innovation* in the environmental molecular sciences to support the needs of DOE and the nation.



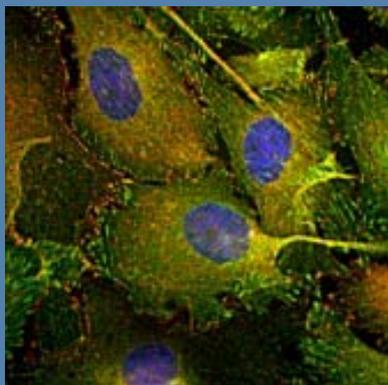
What EMSL offers

- ◆ Unique collection of world-class capabilities
 - Catalysis and computational chemistry
 - Systems biology
- ◆ Free use for published/open research
- ◆ 50% of users from academia
- ◆ More than 700 users last year, either accessing capabilities on site or remotely



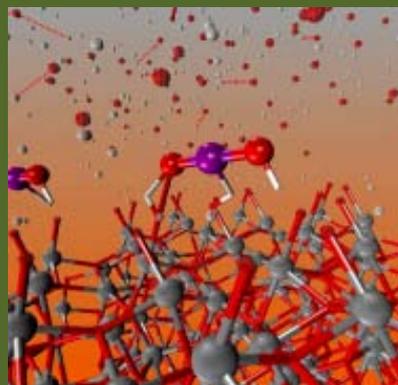
The user program is focused on three Science Themes

Biological Interactions and Dynamics



Understanding and optimizing the response of biological systems to their environment.

Geochemistry/Biogeochemistry & Subsurface Science



Unraveling molecular-level phenomena to fate and transport in the subsurface.

Science of Interfacial Phenomena

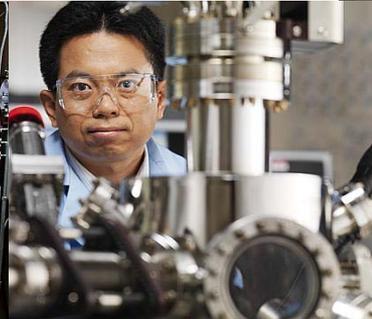
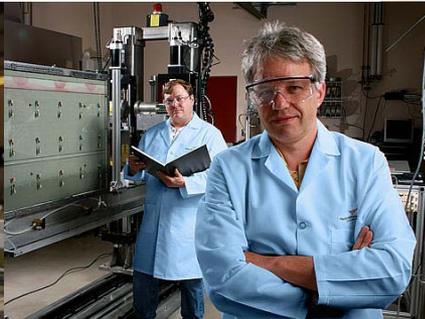
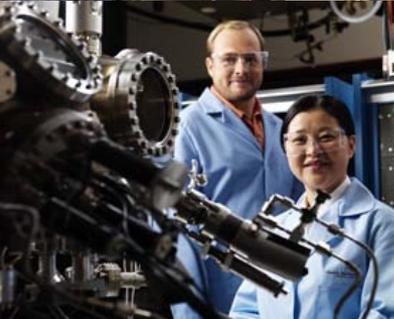


Developing an advanced understanding of structure-function relationships in catalysis.

Integration sets EMSL apart



- EMSL staff excel at coupling instrumentation & techniques for greater impact
- Unique collection of instruments enables new approaches
- Expert EMSL staff work closely with users to accelerate innovation



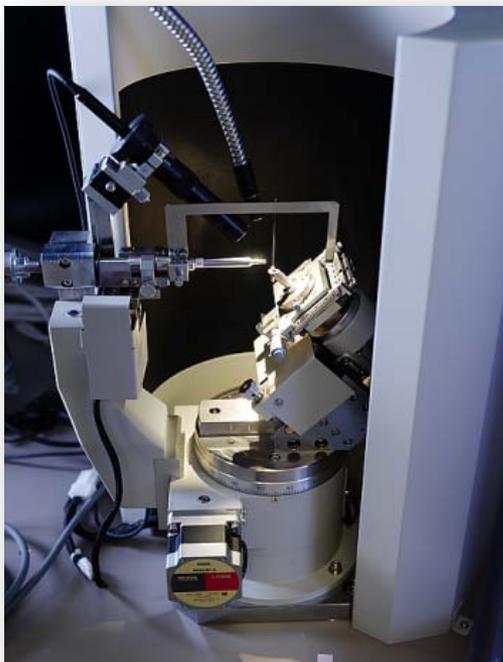
Full capability suite at EMSL




Pacific Northwest
NATIONAL LABORATORY



Proudly Operated by **Battelle** Since 1965



- Surface science and modeling
 - ◆ X-ray photoelectron spectroscopy
 - ◆ X-ray fluorescence
 - ◆ Scanning and transmission electron microscopy
 - ◆ X-ray diffraction
 - ◆ Nuclear magnetic resonance (NMR)
- Computational science
 - ◆ 163-teraflop Chinook supercomputer
 - ◆ NWChem



Biotechnology capabilities to accelerate biomass advancements

- Proteomics & metabolomics
 - ◆ High-throughput mass spectrometers
- Nuclear magnetic resonance (NMR)
- Electron paramagnetic resonance
- Microscopy
- Next-generation sequencers for transcriptome analysis
- Cell isolation



Examples of Catalysis & Computational chemistry

Characterization of catalysts assists new process for biofuels



Value to biomass:

Waste wood products are a potential source of ethanol as alternative fuel but not yet economically viable

Study:

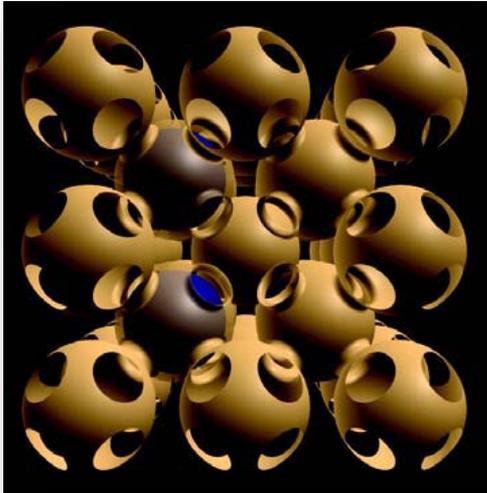
Understand how a catalyst changes over time – and specifically, how to increase its useful life and selectivity – in converting waste wood products to ethanol. Through CRADA with private biomass conversion company.

Methods used:

Characterizing the catalyst as it's used over time, correlating structure to catalyst function, modeling catalyst behavior from first principles.

Users:

Mark Engelhard and team, EMSL
Mark Lilga, PNNL



Value to biomass:

Optimizing efficient, regenerable catalysts leads to enhanced removal of pollutants at lower costs. Syngas is produced in the gasification of biomass, and thus helps meet the demand for cleaner transportation fuels.

Study:

- Evaluate effectiveness of one catalyst's use of its cage-like 3-D structure to protect metal and metal oxide particles from heat damage
- Create new class of SBA-16-supported regenerable metal catalysts that remove unwanted sulfur from syngas fuel

Methods used:

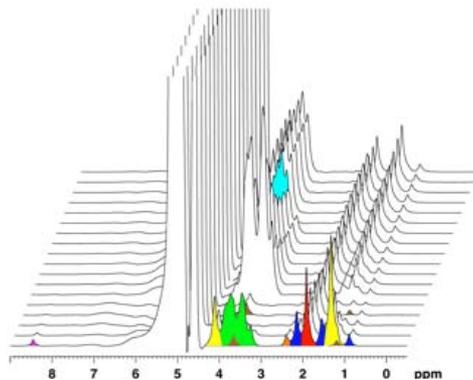
High-resolution transmission electron microscopy

Users:

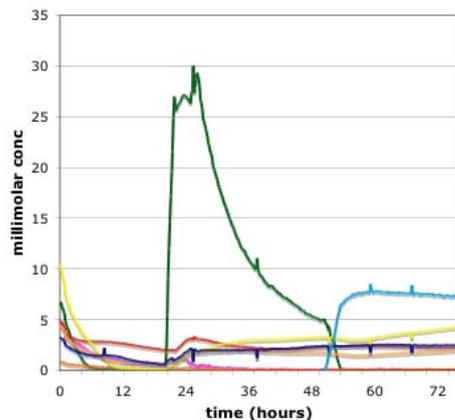
Yong Wang of PNNL and Washington State University

Examples of Biotechnology

Developing insights to metabolomics for bioproduct development



— formate — glucose
— lactate — ethanol



— pyruvate — acetate
— n-butyrate — fructose

NMR time-series data (above) and derived metabolite concentrations (below) for a *Eubacteria aggragens* suspension .

Value : Understanding microbial metabolism (metabolic profiles, pathways and flux rates) provides insight to optimize bioproduct yields

Study:

Analyze metabolism of anaerobic thermophiles relevant to biofuel production

Methods used:

EMSL's unique NMR bioreactor enables *live, in-situ metabolic* studies. Combined with state-of-the-art high-resolution NMR and LC-NMR, provides more accurate metabolic profiles

Users:

Paul Majors, PNNL
Nancy Isern, EMSL

Identifying proteins critical to cellulose digestion



Value to biomass:

Bacteria's potential role in cellulose digestion provides potential to identify novel proteins with applications toward biofuel & antibiotic development

Study:

Symbiotic relationship of leafcutter ants, fungi & bacteria

Methods used:

JGI: Sequencing of metagenome of fungus garden

EMSL: Identification of protein abundances and distributions within bacterial community

Users:

Cameron Currie of UW-Madison and Great Lakes Bioenergy Research Center

Analyzing enzymes to study potential to degrade lignocellulose



(photo by DOE Joint Genome Institute)

Value to biomass:

Enhance understanding of potential value for bacterial communities found in a termite's 'hindgut' to degrade lignocellulose

Study:

Costa Rican termite gut

Methods used:

JGI: Metagenomic analyses conducted

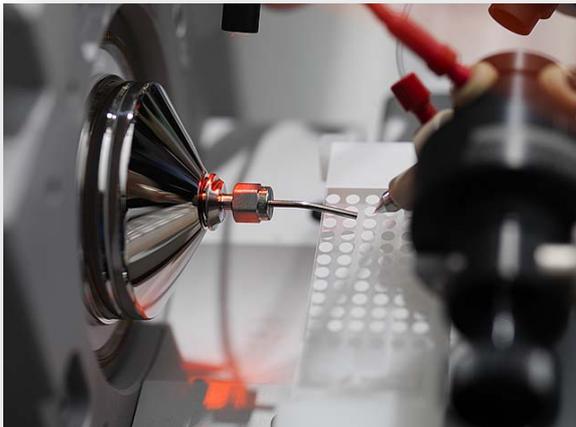
EMSL: Metaproteomic analyses conducted to gain insight into hypothesized symbiotic mechanisms, including: cellulose/hemicellulose degradation and fixation of atmospheric nitrogen gas.

Users:

Philip Hugenholtz, DOE JGI

Falk Warnecke, LBNL

Rudolf H Scheffrahn, University of Florida

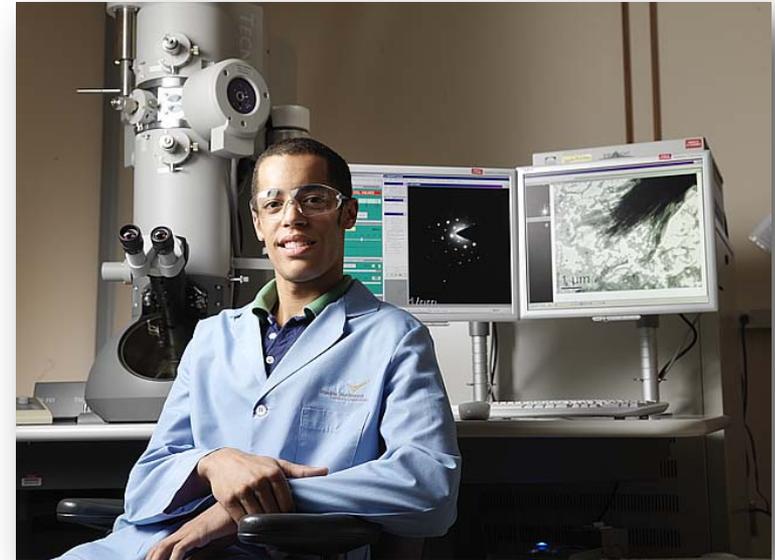


ARRA investments leading to new instrumentation for biomass

- Improved microscopy/imaging
- Proteomics/metabolomics
- Catalysis
 - ◆ 850-MHz wide bore NMR for catalysis
 - ◆ *In-situ* aberration-corrected transmission electronic microscopy
- Transcriptomics
 - ◆ Transcriptional Profiling using Next-Generation Sequencing Technology (RNA-Seq)
 - ◆ Cell sorter
- High Resolution mass spectrometer
 - ◆ Microbial community proteomics
 - ◆ Advanced biofuel and petroleum characterization



- Science Theme
 - ◆ Up to three years
 - ◆ Submitted via a proposal call
- Partner
 - ◆ Cost sharing
 - ◆ Capability building
 - ◆ Submitted at any time
- Rapid
 - ◆ Up to 1 month
 - ◆ Submitted at any time
- General
 - ◆ Up to 1 year
 - ◆ Submitted at any time
- Capability based
 - ◆ Up to 2 years
 - ◆ Submitted via proposal call.



Latest call for proposals
opened March 8
Closes April 8

Proposals are submitted via EMSL's
website – visit user portal
www.emsl.pnl.gov/access

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