Biomolecular Science

The research goal of NREL's Biomolecular Science is to enable cost-competitive advanced lignocellulosic bio-fuels production by understanding the science critical for overcoming biomass recalcitrance and developing new product and product intermediate pathways.
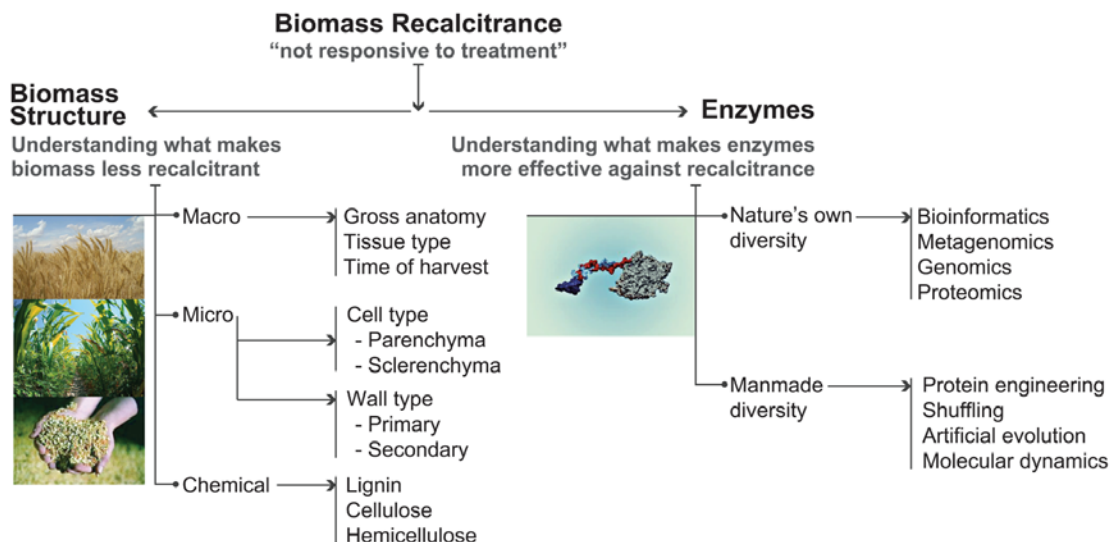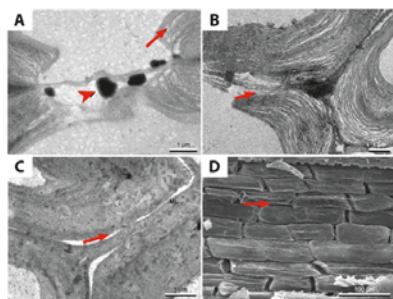
Capabilities

Biomass Structure
- Biomass pretreatment chemistry
- High through-put biomass digestibility screening
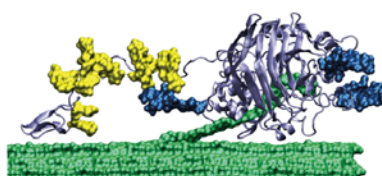- Nanoscale biomass structural characterization.

Enzymes
- Fungal molecular biology
- Enzyme engineering, purification, and assays
- Macromolecular dynamics and simulation.

Biomass Recalcitrance
"not responsive to treatment"

Biomass Structure ← → **Enzymes**

Understanding what makes biomass less recalcitrant

Understanding what makes enzymes more effective against recalcitrance

- Macro → Gross anatomy / Tissue type / Time of harvest
- Micro → Cell type - Parenchyma - Sclerenchyma / Wall type - Primary - Secondary
- Chemical → Lignin / Cellulose / Hemicellulose

- Nature's own diversity → Bioinformatics / Metagenomics / Genomics / Proteomics
- Manmade diversity → Protein engineering / Shuffling / Artificial evolution / Molecular dynamics
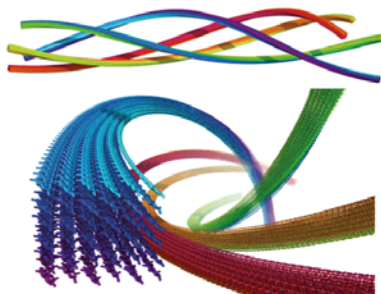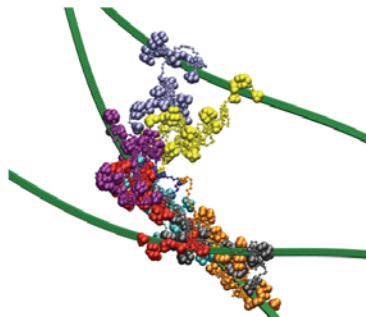
Research Highlights

Pretreatment of switchgrass changes cell wall architecture to improve digestibility. Micrographs showing the impact of thermochemical pretreatment on delaminating cell walls and increasing porosity. (A) Pretreatment delaminated secondary cell wall, particularly near cell pits (arrow). (B) Extensive delamination throughout the cell walls (arrow). (C, D) Pretreatment separated adjacent cells by disrupting and dissolving the middle lamella (arrows).

The *O-glycosylated linker* from the *Trichoderma reesei* Family 7 cellulase is a flexible, disordered protein. Cel7A from *Trichoderma reesei* on cellulose. The enzyme is shown in purple, the O-glycosylation on the linker is in yellow, and the N-glycan on the CD is in blue. Cellulose is in green, with a single cellodextrin chain threaded into the CD tunnel.

Atomistic, macromolecular models of cellulose microfibrils. The macromolecular geometries extracted from the tomographic data were used to generate atomistic models for cellulose microfibrils based on the 1β crystal structure polymorph. The twist of the fibrils was inferred from the macromolecular geometry by orienting the structures such that the bending about the 010 plane of the crystal structure was minimized.
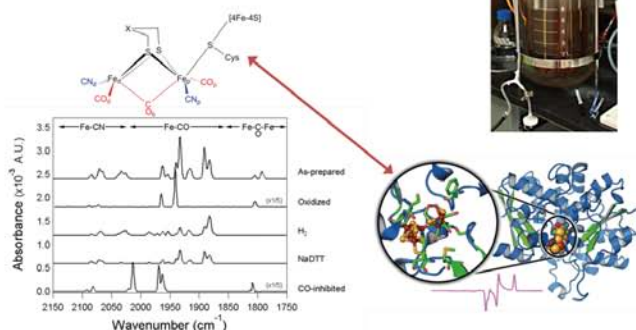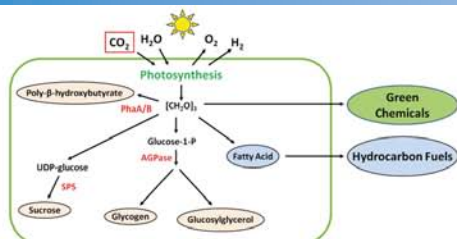

Modeling the self-assembly of the cellulosome enzyme complex. Simulation of a large cellulosome acting on several cellulose microfibrils (green). In cellulosomes, cellulases are arranged on a protein scaffold as opposed to fungal cellulases that are free enzymes.

NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

Photobiology

NREL's Photobiology focuses on understanding the capture of solar energy in photosynthetic systems and its use in converting carbon dioxide and water directly into hydrogen and advanced biofuels.
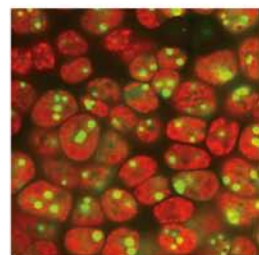
Capabilities

- Metabolic pathway engineering in algae/bacteria/cyanobacteria
- Advanced photobioreactors
- Large-scale protein production for characterization of enzymes
- Structure/function relationship in metalloenzymes that catalyze H_2 production using biophysical tools such as infrared spectroscopy
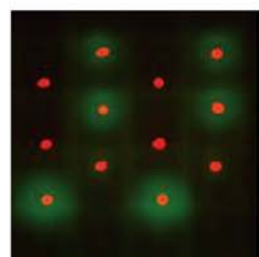- Continuous fermentation for biofuels production

Research Highlights

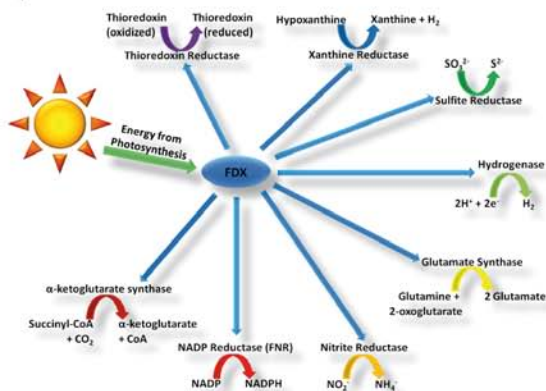**Visualization of biofuels-producing algal cells with colorimetric sensors**

Algal cells (red) stained with a green dye (BODIPY) identifying accumulation of lipids (a valuable fuel precursor)
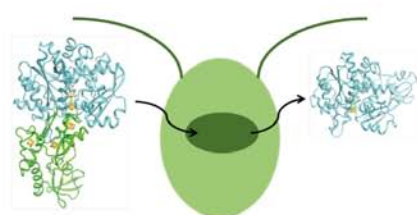
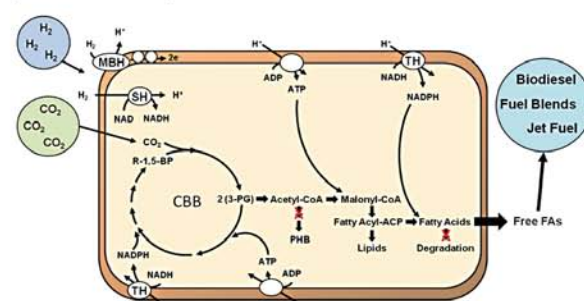H_2 and non-H_2 producing algae (red) identified with a biological H_2 sensor (green)

Fundamental studies of energy flow from photosynthesis to important biochemical reactions including hydrogen production

Replacement of algal hydrogenases with a bacterial hydrogenase for increased oxygen tolerance

Uptake and utilization of renewable H_2 and carbon dioxide (CO_2) in a novel, engineered micro-organism that directly produces a variety of fuel substitutes

Solar-driven hydrogen production via artificial photosynthesis