U.S. DEPARTMENT OF ENERGY

# Center for Lignocellulose Structure and Formation

## an Office of Basic Energy Sciences
## *Energy Frontiers Research Center*


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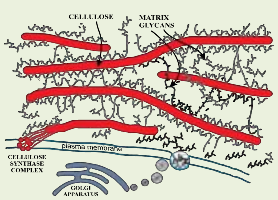
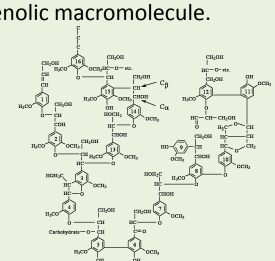
**Lignocellulose** is the major structural material of plant bodies and constitutes the enormously important biorenewable resource used to make building materials, paper, textiles and many polymer derivatives. Lignocellulose is also the largest store of renewable solar energy on Earth, but its structure presents a major impediment to conversion into useful forms of transportation fuel. CLSF is a 5-year, $21M Center (Penn State is lead institution) funded by DOE to investigate lignocellulose structure and formation.

***Center Objective: To dramatically increase our fundamental knowledge of the physical structure of bio-polymers in plant cell walls to provide a basis for improved methods for converting biomass into fuels.***

At the nanoscale lignocellulose is a highly versatile composite of three complex biopolymers, namely, crystalline nm-scale fibrils of cellulose which are linked together by less-ordered polysaccharides (such as xylans) and embedded in lignin, a complex and heterogeneous phenolic macromolecule.



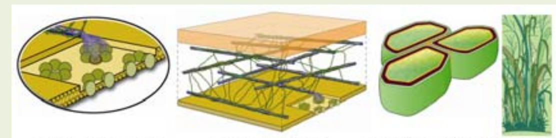



*Above, left: Cellulose is spun out as a nm-scale microfibril from a synthase complex in the plasma membrane whereas matrix glycans are packaged in membrane-bound vesicles which deposit them to the cell surface. Thereafter they bind to cellulose. Above, right: Representative structure of lignin, which impregnates the spaces between cellulose microfibrils.*

Work in the CLSF center is organized around three questions:
*(1) How does the cellulose synthase complex produce the cellulose microfibril?*
*(2) What are the physicochemical interactions among cell wall components that lead to a strong network and what are the steps in their assembly?*
*(3) How do macro-scale properties of cell walls (mechanics, porosity, thermal properties, etc.) emerge from nano-scale properties of cell wall components?*

## Some common forms of lignocellulose:

**Three themes of the Center:**




**Theme 1** focuses on CSC, the Cellulose Synthase Complex, and the physical process of cellulose microfibril formation in plant and microbial systems. Specific objectives include solving the structure of cellulose synthase; identifying proteins in the CSC complex; identifying genes that modulate cellulose structure; nanoengineering cellulose synthases into functional forms in nanotubes and nanomembrane arrays; and using computational modeling to explore the cellulose synthase packing within the CSC and the pathway for crystallization of the cellulose microfibril.

**Theme 2** focuses on the structure and assembly of lignocellulose from its constituent components (cellulose, hemicellulose, lignin). Objectives include experimental analysis of the energetics and kinetics of binding of xylans, glucans and lignin to cellulose in its various forms; molecular modeling of the key molecular components of cellulose-matrix binding interactions; developing tractable experimental systems for producing cell walls and artificial cell walls whose structure and composition are readily controlled; and spectroscopic, microscopic and biomechanical studies to elucidate the interactions between cell wall components.

**Theme 3** focuses on the development and validation of a multiscale model that will bridge the basic nano and molecular scale knowledge gathered in themes 1 and 2 to real-world applications including drying and chemical/enzymatic degradation.

CLSF is comprised of an interdisciplinary team that includes plant and microbial molecular biologists, chemists, physicists, material scientists, engineers and computational modelers who will use cutting-edge approaches and methodology to advance our understanding of the "rules of assembly" of the plant cell wall. Investigators include:
- **Pennsylvania State University:** Daniel Cosgrove (Director), Jeffrey Catchmark (Associate Director), Tom Richard, James Kubicki, Ming Tien, Teh-hui Kao, Janna Maranas, John E. Carlson, Virendra Puri, Nicole Brown, Linghao Zhong, Douglas Archibald, Bernhard R. Tittmann, Vincent Crespi.
- **North Carolina State University:** Candace Haigler, Yingling Yaroslava, Alex Smirnov
- **Virginia Tech University:** Alan Esker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