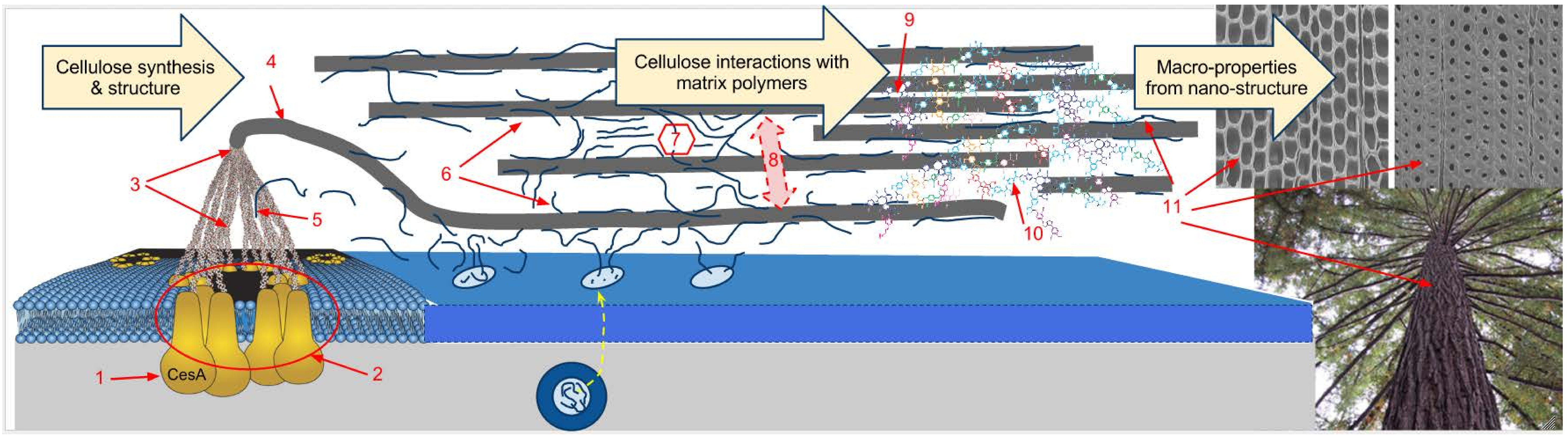
Center for Lignocellulose Structure and Formation

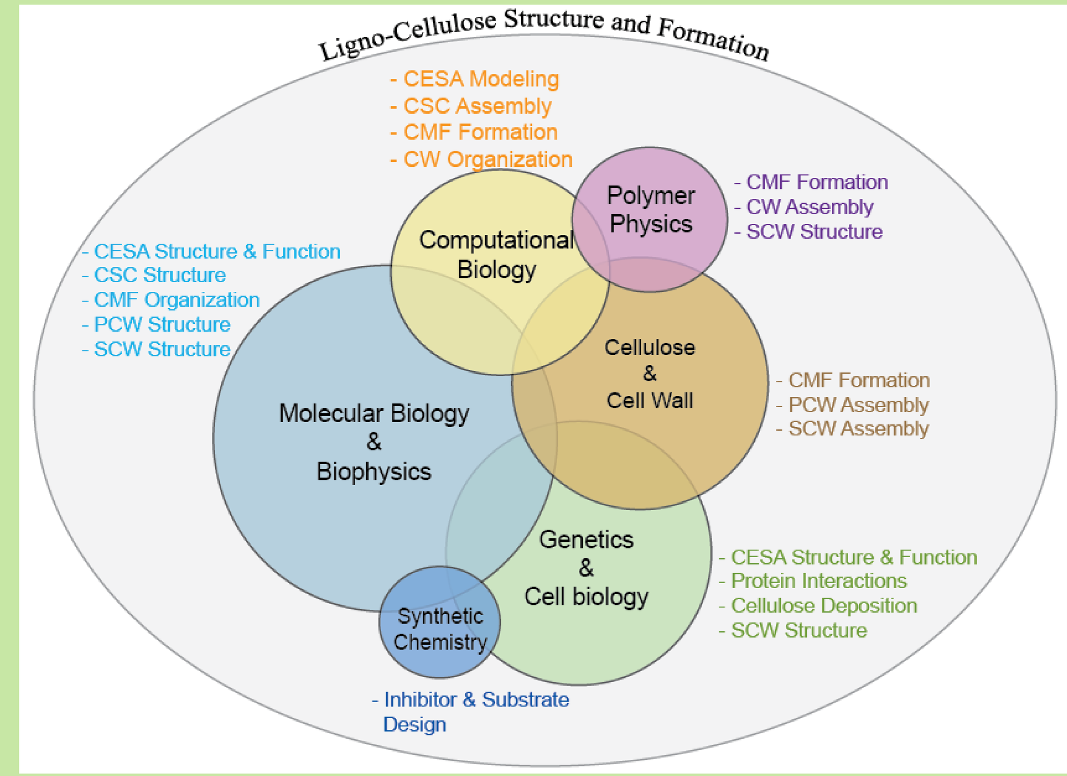
An Energy Frontiers Research Center supported by the US Department of Energy, Office of Basic Energy Sciences



CLSF Mission

To develop a nano-scale understanding of the structure and formation of lignocellulose, the main structural material in plants, forming a foundation for significant advances in sustainable energy and materials.

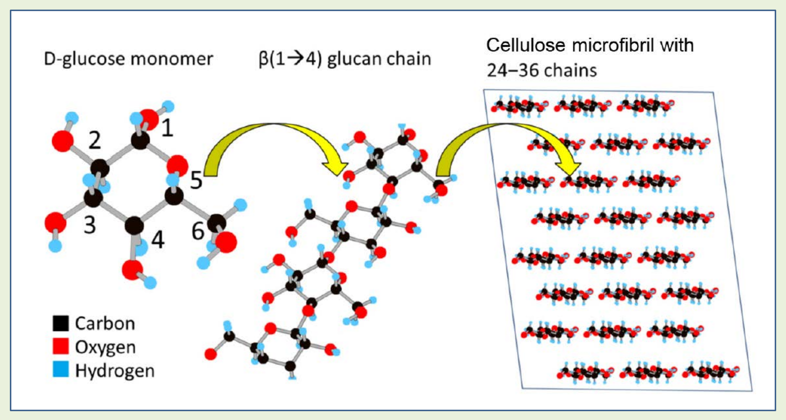
Collaborative, integrated transdisciplinary research



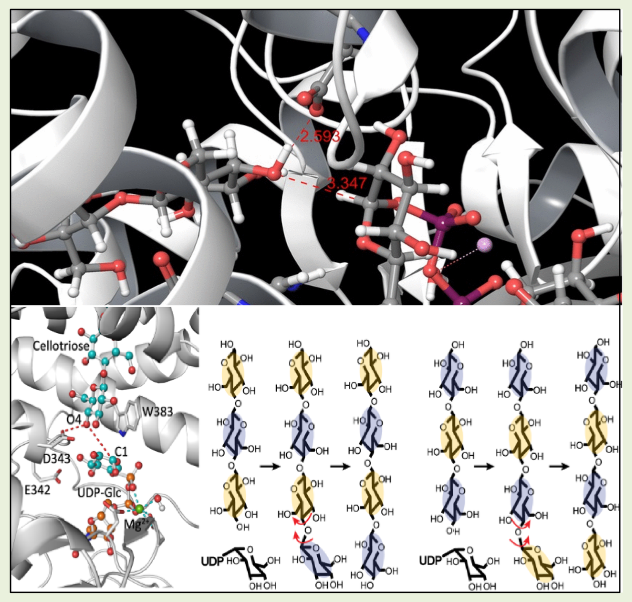
The CLSF brings together unique expertise to reveal how plants construct their cell walls. Our goals are to discover how cellulose microfibrils are synthesized in diverse forms and how plant cell wall properties, including recalcitrance, emerge from interactions and assembly of cell wall polymers.

Theme 1: How plants make cellulose:

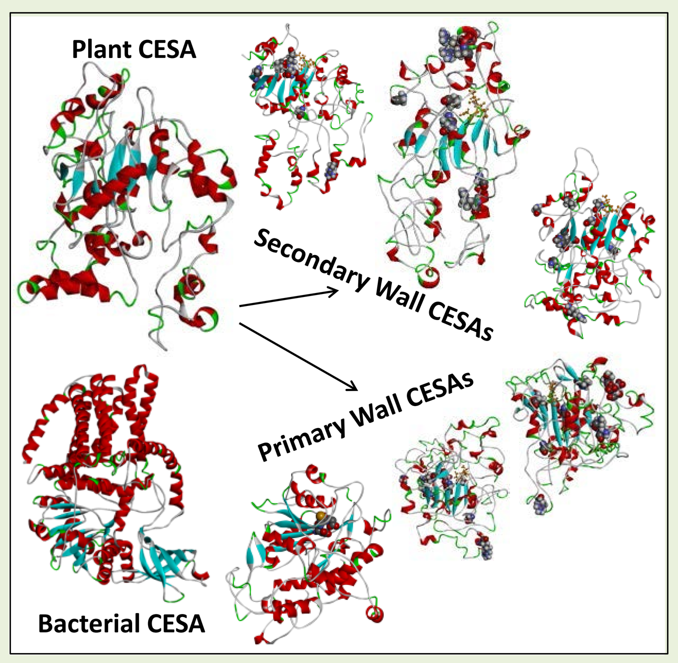
- **Structure and function of cellulose synthase (CESA)**
- **Structure and function of cellulose synthesis complex (CSC)**
- **Regulation of CSC activity and cellulose fibril formation**



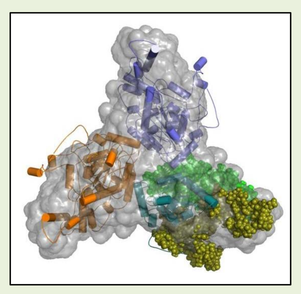
Chemical structures of D-glucose, glucan chain and cross section of cellulose microfibril (Kim 2013)



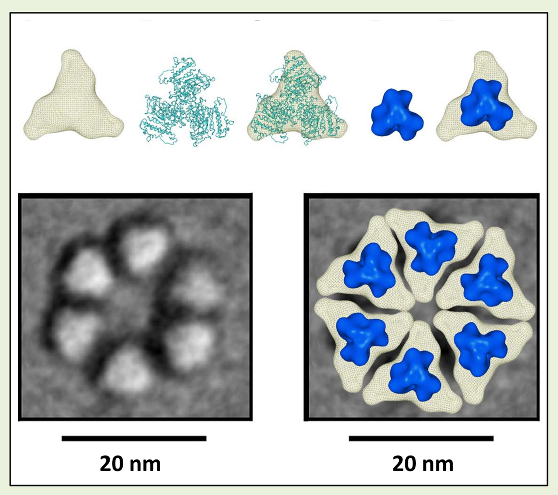
QM/MM analysis provides the first theoretical model of the mechanism by which cellulose synthase elongates a cellulose polymer one glucosyl moiety at a time (Yang et al. 2015)



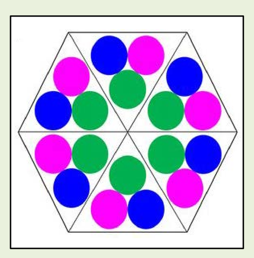
Structure prediction of individual CESAs (Y Yingling, NCSU)



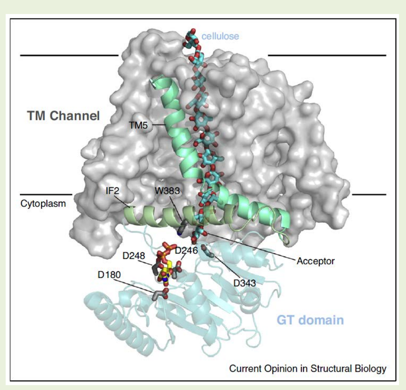
Ab initio model of ATCESA1catD trimer overlaid with ROSETTA model. P-CR and CSR regions are shown in green and olive spheres (H O'Neill, ORNL)



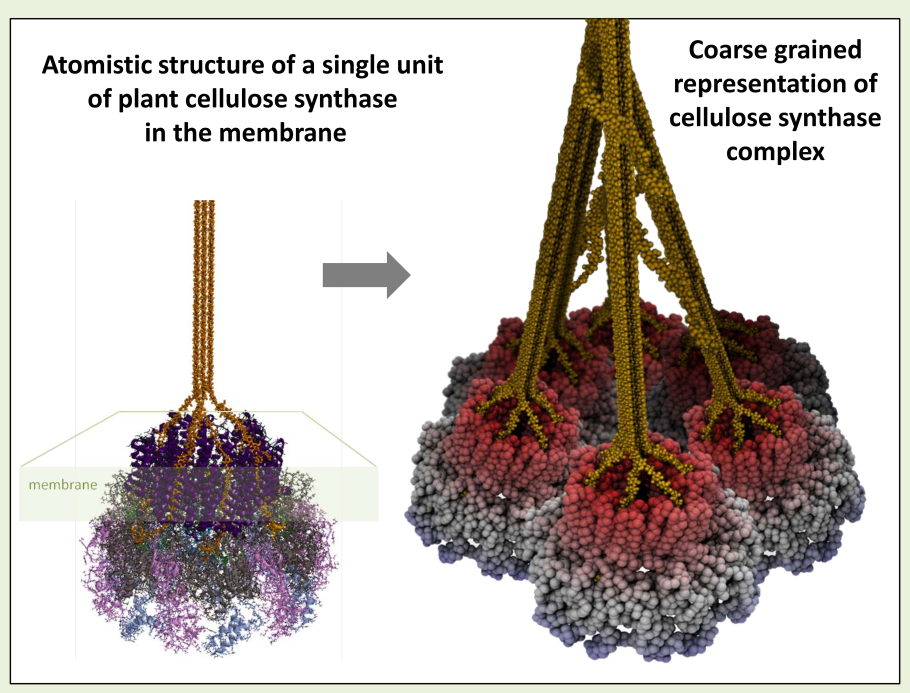
Modern image analysis is used to determine number and arrangement of CESAs in CSCs: Trimer of Pp TMH region is consistent with proven trimers of cytosolic domain of AtCESA (BT Nixon, H O'Neill, C Haigler, PSU, ORNL and NCSU)



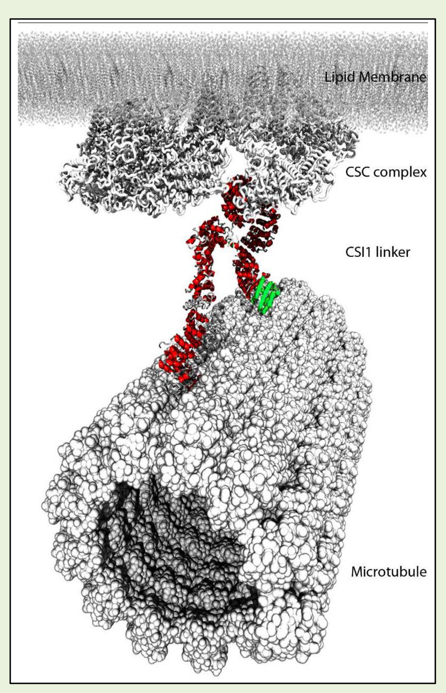
Current model for the CSC as a hexamer of CESA hetero-trimers (Hill et al. 2014)



Pore organization of bacterial cellulose synthase subunit BcsA with cellulose chain (Bi et al. 2015)



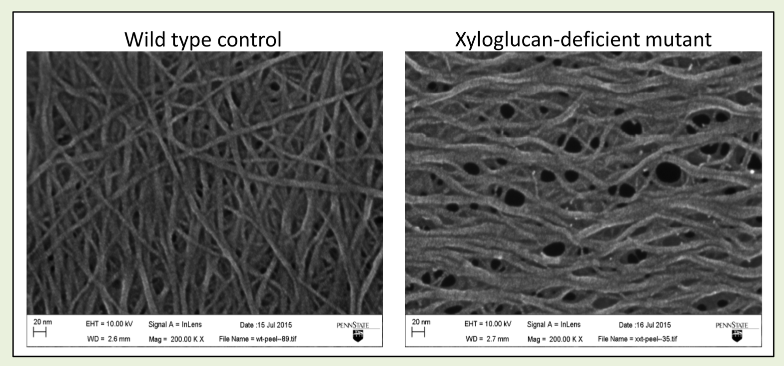
In silico models of plant CSC structure and cellulose microfibril formation (Y Yingling, NCSU)



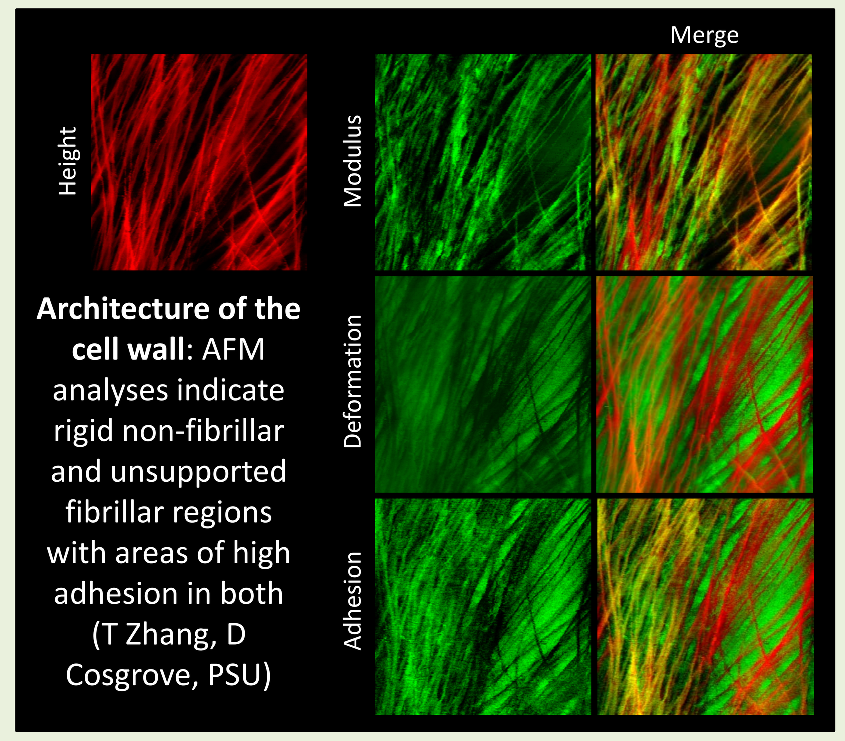
Putative interaction of cellulose synthase interactive protein1 (CSI1) with CSC complex and microtubule (Lei et al. 2015)

Theme 2: How plants assemble multi-functional cell walls:

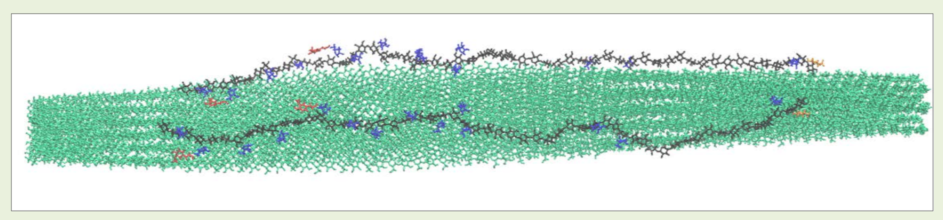
- **Mesoscale architecture of the cell wall**
- **Polymer interactions and conformations**
- **NMR of primary and secondary walls, including grasses**
- **Matrix polymer delivery**
- **Mobility of water, polysaccharides and proteins in the wall**
- **Coarse grain model of the primary cell wall**
- **Macrofibril formation and lignification (secondary cell walls)**
- **Spectral analysis of cell wall structure**



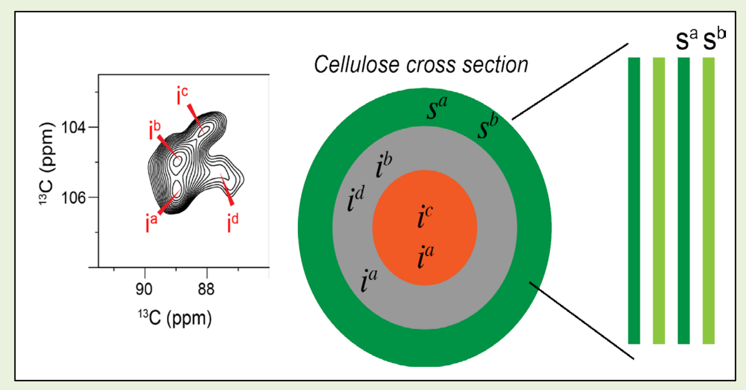
Mesoscale architecture of cell wall: Lack of xyloglucan shows enhanced alignment of cellulose as imaged with FESEM (Y Zheng, C Anderson, D Cosgrove, PSU)



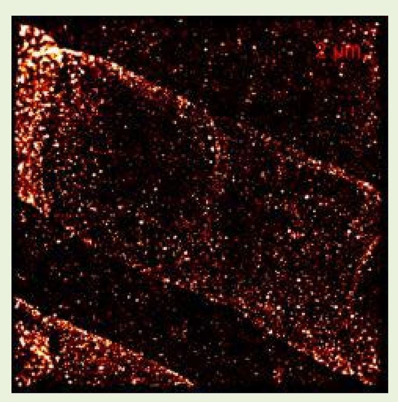
Architecture of the cell wall: AFM analyses indicate rigid non-fibrillar and unsupported fibrillar regions with areas of high adhesion in both (T Zhang, D Cosgrove, PSU)



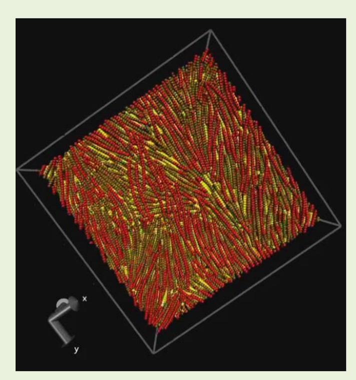
Polymer interactions and conformations: Characterizing the association between glucuronoarabinoxylan and cellulose in the plant cell wall (S Smith, L Petridis, D Cosgrove, ORNL and PSU)



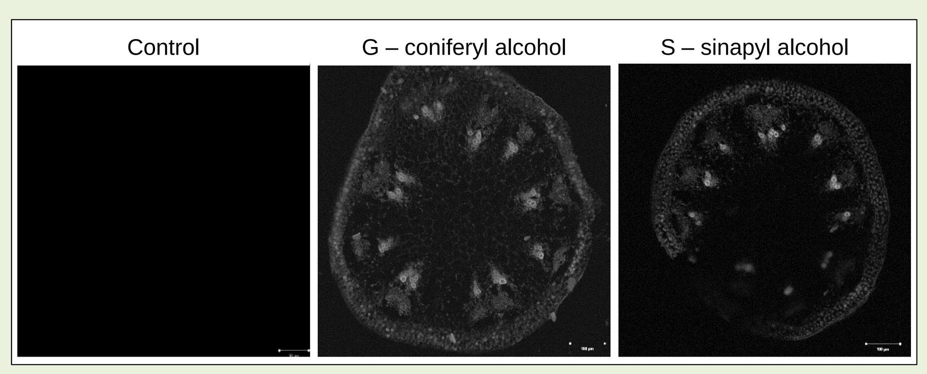
NMR of primary and secondary walls, including grasses: Proposed locations of different cellulose forms in the plant cell wall microfibril (T Wang, M Hong, MIT)



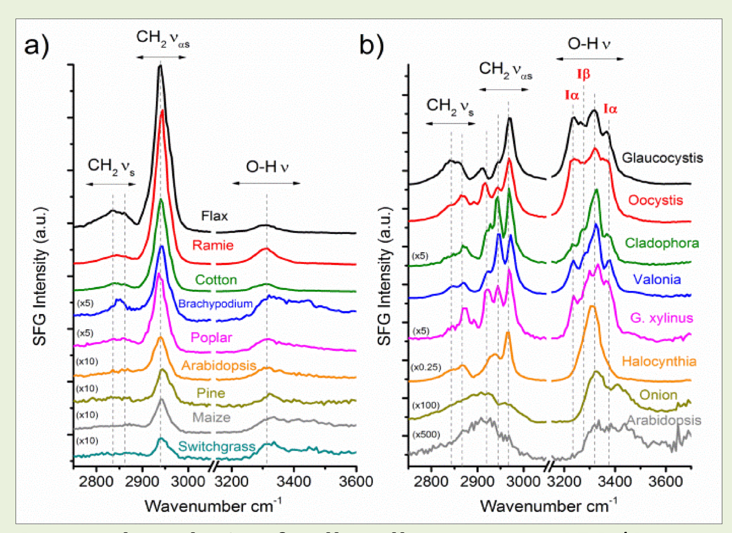
Matrix polymer delivery: Alkynyl fucose clickable probes for metabolic labeling and fluorescence imaging of polysaccharides (pectin) in cell walls (D McClosky, C Anderson, PSU, and R Dalrymple, Zeiss)



Coarse grain model of the plant cell wall: Microfibril beads in exemplary simulations: color-coded by the position along the Z-axis (M Kowilak, J Maranas, PSU)



Lignification (secondary cell walls): Incorporation of different monolignols in Arabidopsis stem sections (S Kiemle, D Cosgrove, PSU)



Spectral analysis of cell wall structure: SFG (Sum Frequency Generation) spectra of cellulose in biological tissues (Lee et al. 2014)

CLSF Lead Institution

PennState

Partner Institutions

MIT
NC State University
Oak Ridge National Laboratory
University of Rhode Island
University of Virginia

Director
Daniel J. Cosgrove (Biology, PSU)

Associate Director
Candace Haigler (Crop Sci & Plant Bio, NCSU)

Senior Investigators
Charles T. Anderson (Biology, PSU)
Ying Gu (Biochem & Mol Biol, PSU)
Seong Kim (Chem Eng, PSU)
James Kubicki (Geosciences, PSU)
Manish Kumar (Chem Eng, PSU)
Janna Maranas (Chem Eng, PSU)
Karl Mueller (Chemistry, PSU)
B. Tracy Nixon (Biochem & Mol Biol, PSU)
Ming Tien (Biochem & Mol Biol, PSU)
Yara Yingling (Materials Sci & Eng, NCSU)
Alison Roberts (Biol Sciences, URI)
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Poster prepared by Laura Ullrich (PSU)

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