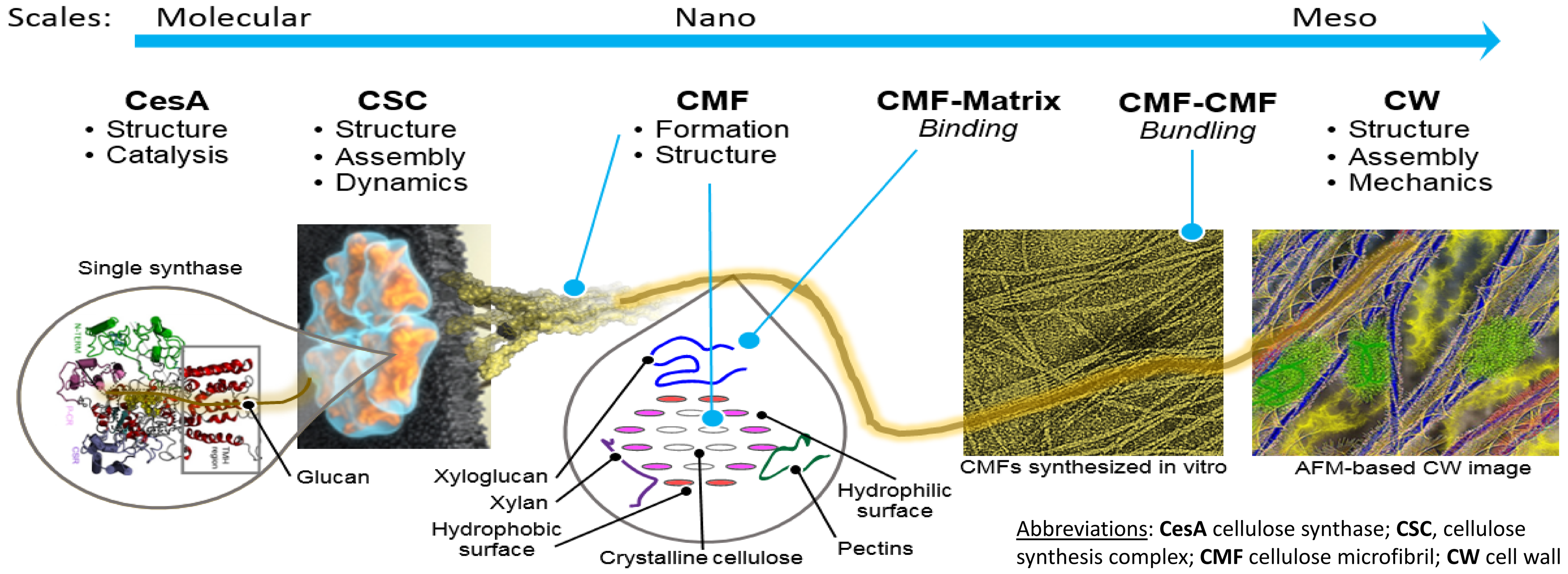
Center for Lignocellulose Structure and Formation

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

CLSF Mission

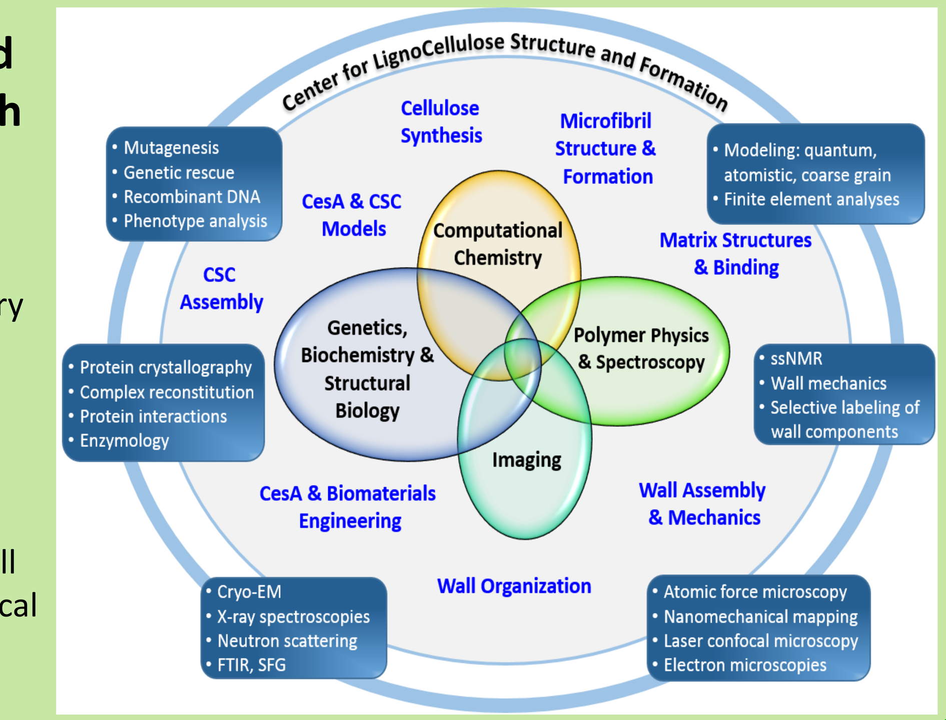
To develop a nano- to meso-scale understanding of plant cell walls, the main structural material in plants, and the physical mechanisms of their assembly, forming the foundation for significant advances in sustainable energy and novel biomaterials.



Abbreviations: **CesA** cellulose synthase; **CSC**, cellulose synthesis complex; **CMF** cellulose microfibril; **CW** cell wall

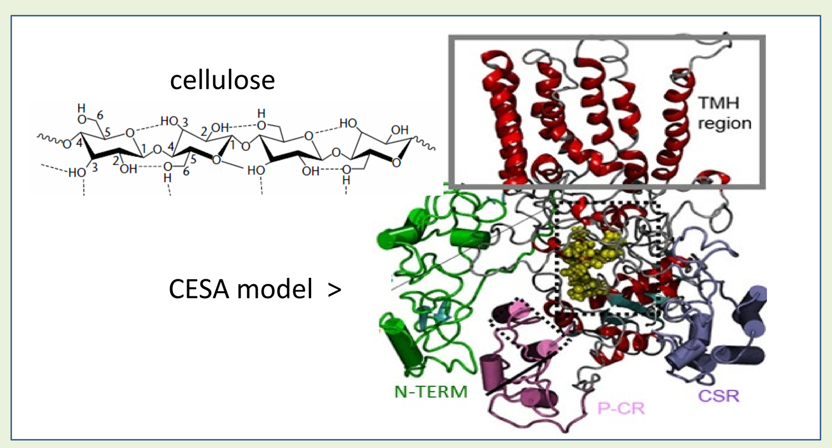
Collaborative, integrated transdisciplinary research

Combining cutting-edge tools of biology and physics, CLSF is elucidating (A) the nano-machinery that transforms simple sugar into cellulose microfibrils and (B) the physical processes by which cellulose interacts with matrix polysaccharides and lignin to produce hierarchically-ordered cell walls with diverse physical, chemical and material properties.

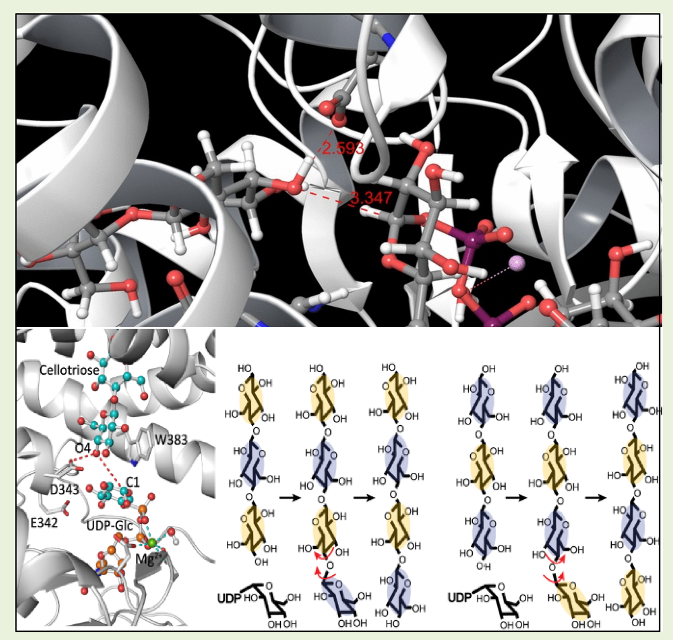


Theme 1: How plants make cellulose:

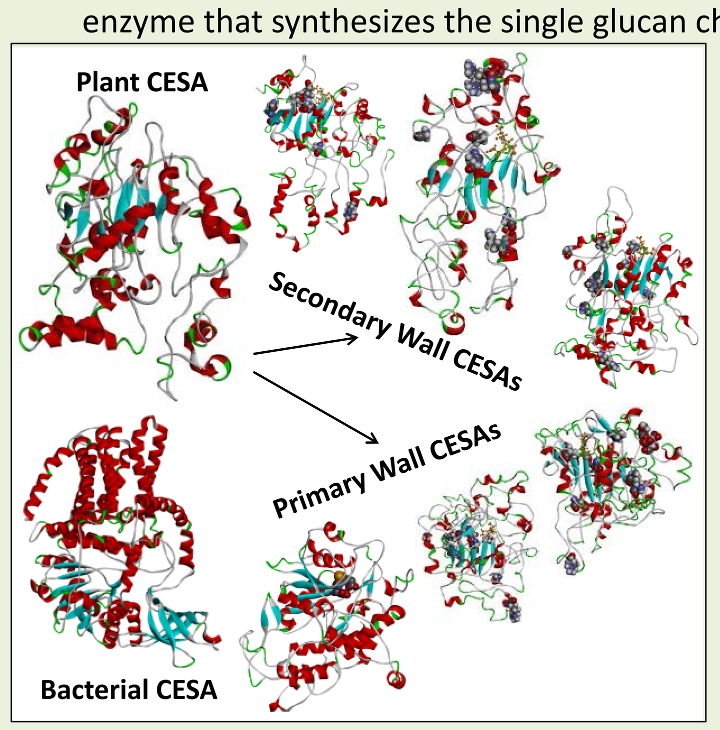
- Structure and function of cellulose synthase (CESA)
- Structure and function of cellulose synthesis complex (CSC)
- Regulation of CSC activity and cellulose fibril formation



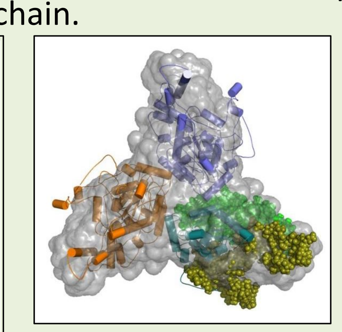
Left: Chemically, cellulose is a polymer of β-1,4-linked D-glucose. Right: CESA is the large multi-domain enzyme that synthesizes the single glucan chain.



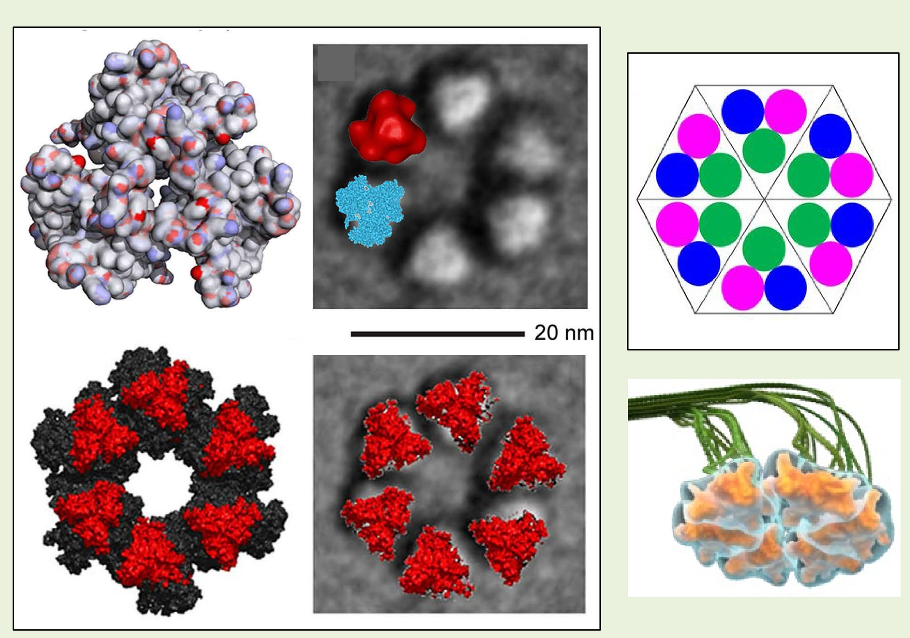
QM/MM analysis provides the first theoretical model of the mechanism by which cellulose synthase elongates a cellulose polymer one glucosyl moiety at a time (Yang et al. 2015)



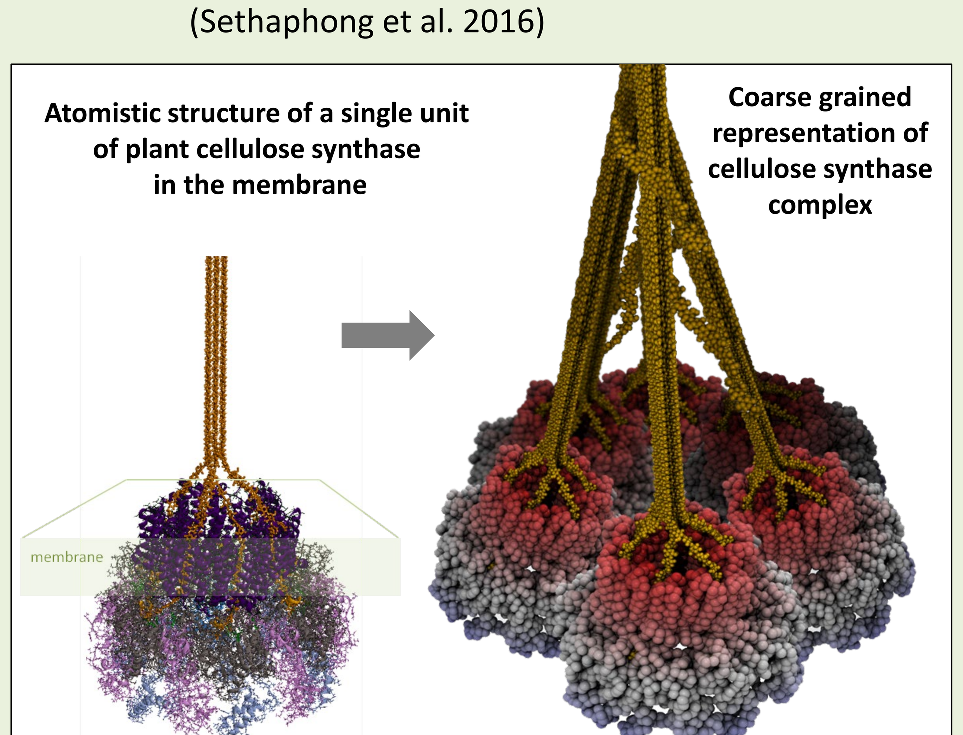
Structure prediction of CESAs isoforms involved in primary and secondary wall formation (Sethaphong et al. 2016)



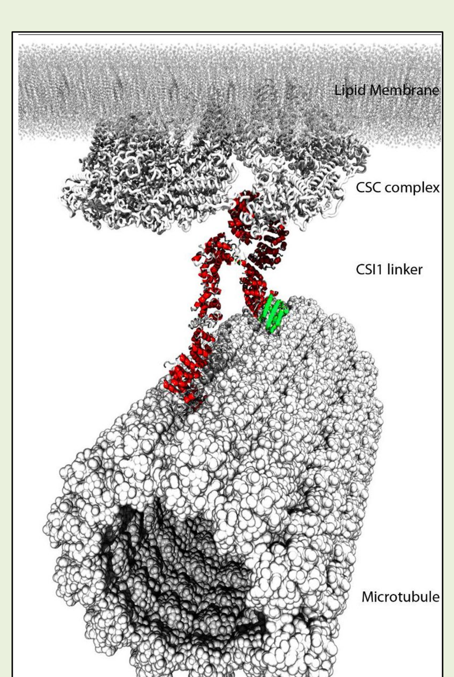
Ab initio model of ATCESA1catD trimer overlaid with ROSETTA model. P-CR and CSR regions are shown in green and olive spheres (Vandavasi et al. 2016)



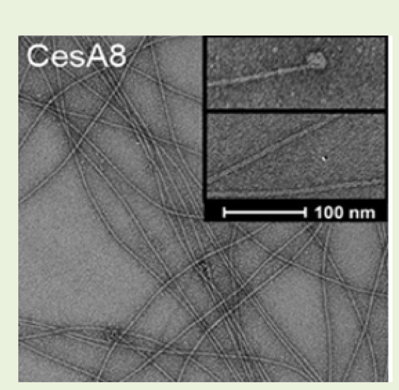
An estimated 18 CESAs are packed in the CSC that produces a cellulose microfibril. A trimer of CESAs packs each of six hexameric subunits of a CSC (predicted using computation and modern image analysis; Nixon et al. 2016, Vandavasi et al. 2016).



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



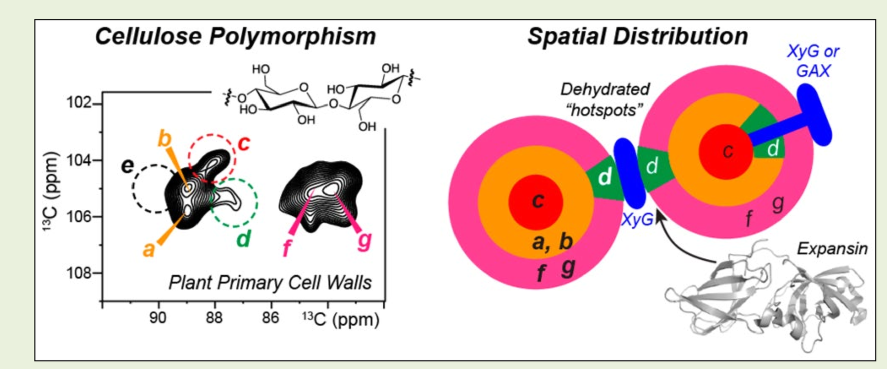
Model of CSI1 protein linking a CSC and a microtubule (Lei et al. 2015)



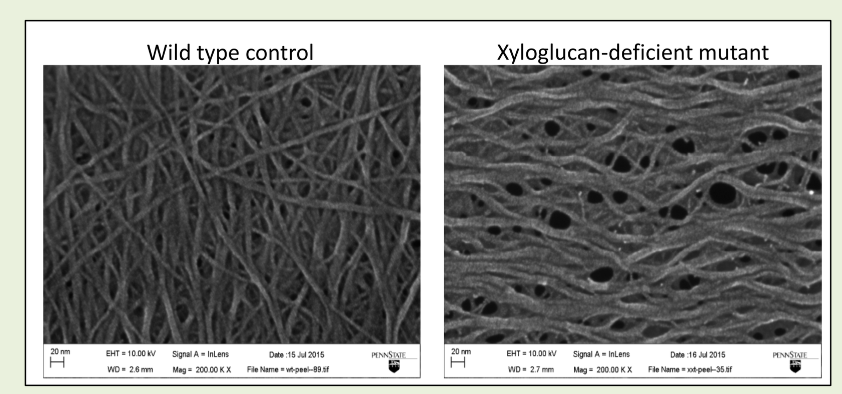
Cellulose microfibrils synthesized in vitro by single CesA isoforms. This shows that a single CesA isoform is catalytically active in the absence of any other plant-derived components and can form microfibrils (Purushotham et al. 2016)

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

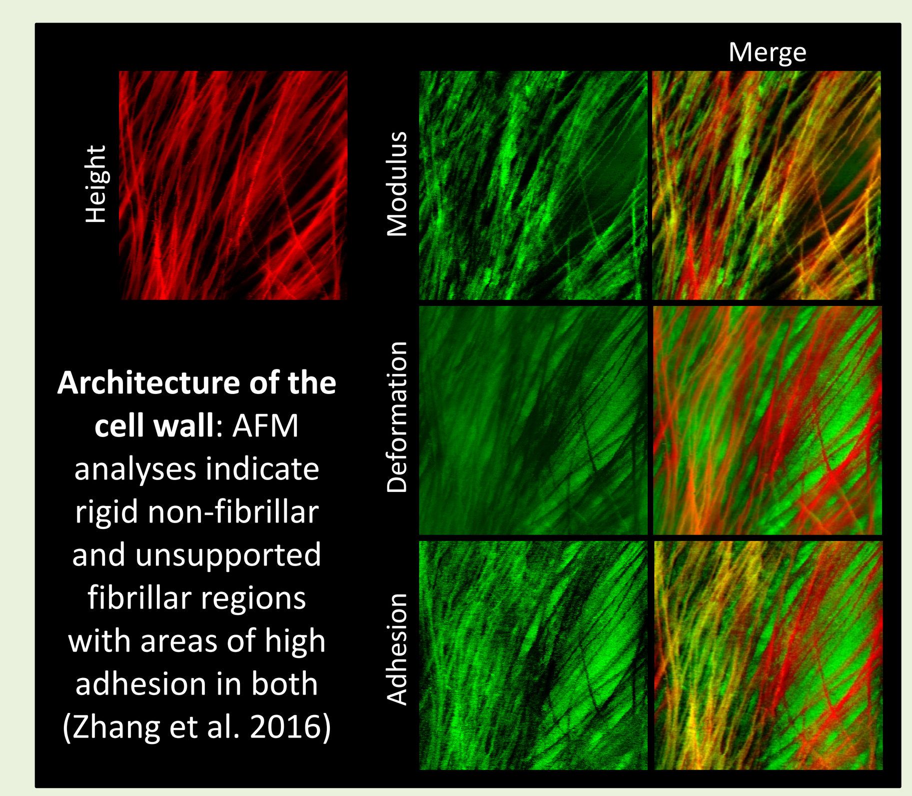
- Mesoscale architecture of the cell wall
- Polymer interactions and conformations
- NMR of primary and secondary walls, including grasses
- Mobility of water, polysaccharides and proteins in the wall
- Coarse grain model of the primary cell wall
- Macrofibril formation and lignification (secondary cell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



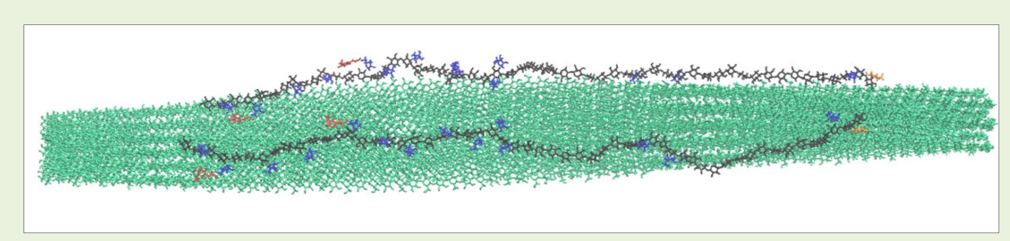
Cellulose structure: ssNMR and density functional theory (DFT) calculations indicate cellulose polymorphism in primary cell walls (Wang et al. 2016)



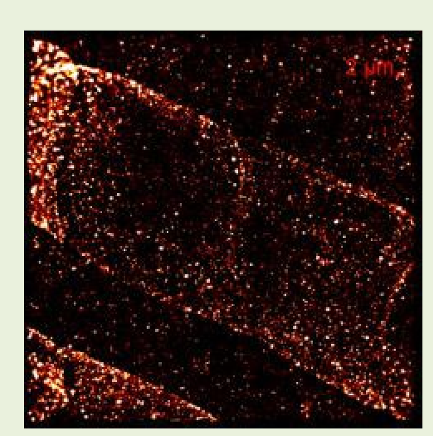
Mesoscale architecture of cell wall: Lack of xyloglucan shows enhanced alignment of cellulose, as imaged with FESEM (Xiao et al. 2016)



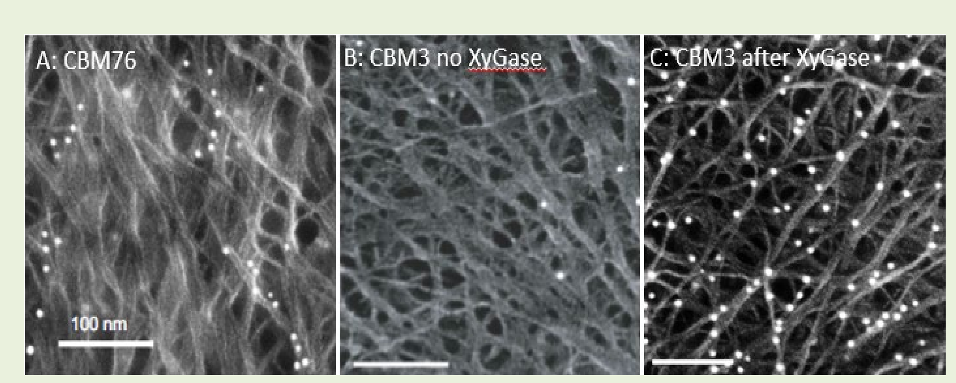
Architecture of the cell wall: AFM analyses indicate rigid non-fibrillar and unsupported fibrillar regions with areas of high adhesion in both (Zhang et al. 2016)



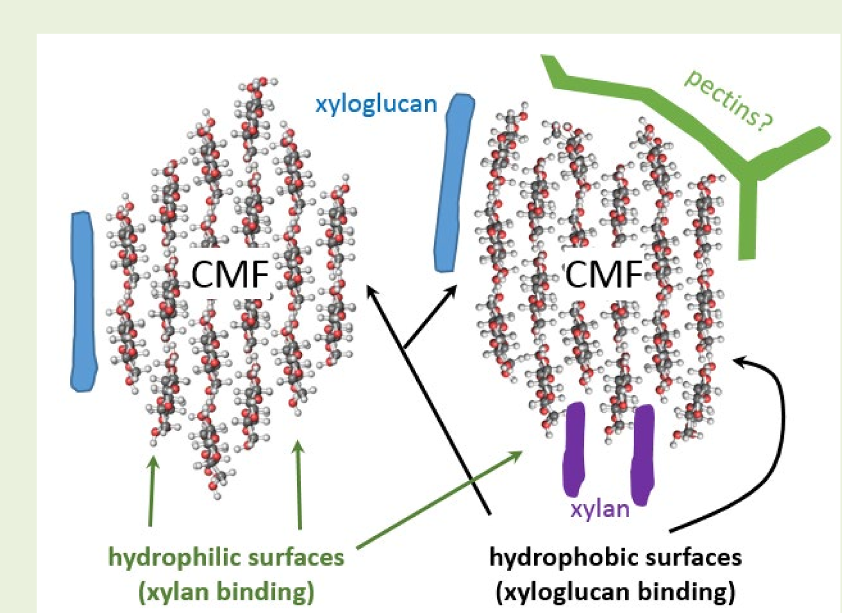
Polymer interactions and conformations: Characterizing the association between glucuronoarabinoxylan and cellulose in the plant cell wall (S Smith, L Petridis, D Cosgrove)



Matrix polymer delivery: Alkynyl fucose clickable probes for metabolic labeling and fluorescence imaging of polysaccharides (pectin) in cell walls (McClosky et al. 2016)



Xyloglucan localization by FESEM with backscattered electron detection. A: CBM76-nanogold reveals xyloglucan position and conformation. B, C: CBM3-nanogold experiments show that xyloglucan is bound to the surface of cellulose. Zheng et al. 2018



Potential arrangements of xyloglucan and pectin at different surfaces of cellulose microfibrils (Cosgrove 2018)

CLSF Lead Institution

PennState

Partner Institutions

MIT; Oak Ridge National Laboratory; NC State University; University of Cambridge; University of Rhode Island; UTEP; 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)
Paul Dupree (Biochemistry, U Cambridge)
Enrique & Ester Gomez (Chem Eng, PSU)
Ying Gu (Biochem & Mol Biol, PSU)
Seong H. Kim (Chem Eng, PSU)
Manish Kumar (Chem Eng, PSU)
B. Tracy Nixon (Biochem & Mol Biol, PSU)
Ming Tien (Biochem & Mol Biol, PSU)
Mei Hong (Chemistry, MIT)
James Kubicki (Geological Sci, UTEP)
Hugh O'Neill (Biol & Soft Matter, ORNL)
Alison Roberts (Biol Sciences, URI)
Yara Yingling (Materials Sci & Eng, NCSU)
Jochen Zimmer (Mol Physiol & Biol Physics, UVA)

Advisory Board:
Vincent Bulone (Swedish Royal IT / Biomime)
Markus Pauly (Heinrich-Heine University)
John Ralph (University of Wisconsin, DOE-GLBRC)
Simon Turner (Univ Manchester

Poster prepared by Laura Ullrich (PSU)

Supported under Award # DE-SC0001090 from the Office of Science, Basic Energy Sciences