Combined Analytics and Modeling Probing Polymer-Polymer Interactions Within Secondary Cell Walls leads to better structural insights

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Background

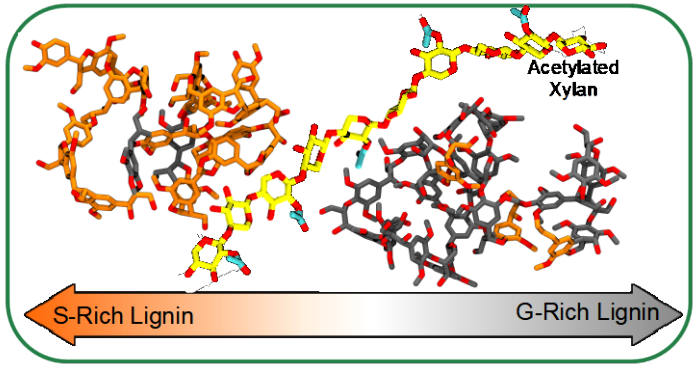
- The molecular-level architecture of the plant Secondary Cell Wall (SCW) is elusive due to the amorphous and heterogeneous nature of lignocellulosic biomass.
- A combined experimental and computational approach is presented to bridge this gap.

Selected Conclusions

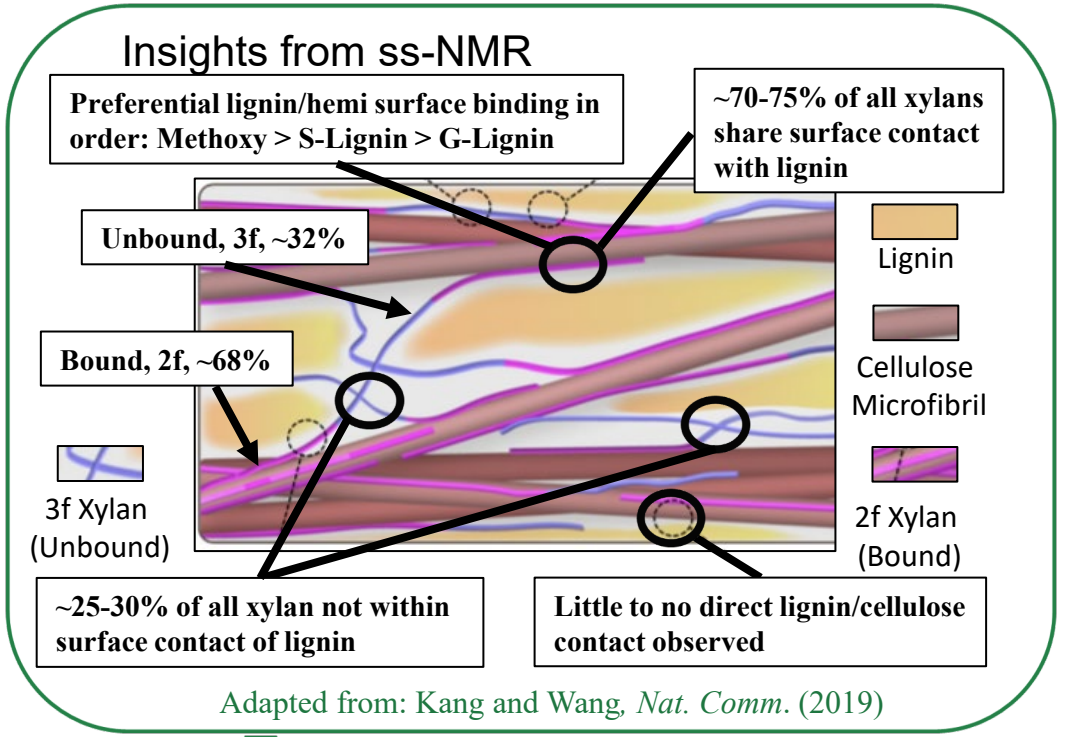
- Polymer-Polymer interactions are probed in detail with solid-state NMR measurements (ssNMR) on ^{13}C-enriched poplar stems.
- Extent of the lignin/hemicellulose interaction is **quantified** for the first time: ~70 – 75% of all acetylated xylan share surface contact with lignin.
- Evidence of preferential xylan/lignin binding: S-lignin > G-lignin.
- Xylan AC_{Me} /Lignin inter-polymer distance is in the order of 0.4 – 0.5 nm
- Molecular dynamics simulations can illuminate the underlying atomistic architectures dictating specific ss-NMR signatures.

Significance

- Investigating plant SCW superstructure using a combined ssNMR and MD approach will greatly improve our molecular-level understanding of cell wall recalcitrance. Experimental data (ssNMR) will inform detailed atomistic cell wall models (MD), together providing better tools capable of predicting deconstruction performance and biomass structure .



Impact of tailored xylan and lignin on ss-NMR observables from MD simulations



Adapted from: Kang and Wang, *Nat. Comm.* (2019)

Informed Molecular Models of the Plant Cell Wall

B. Addison, D. Stengel, V. Bharadwaj R. Happs, C. Doeppke, G. P. Holland, T. Wang, Y. J. Bomble, A. E. Harman-Ware. 2020. ***J Phys Chem B***, DOI:10.1021/acs.jpcb.0c07759 (cover article)
December 2020

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