

Objective 1.1 Science and Technology Results Provide Meaningful Impact on the Field – High Impact Publications

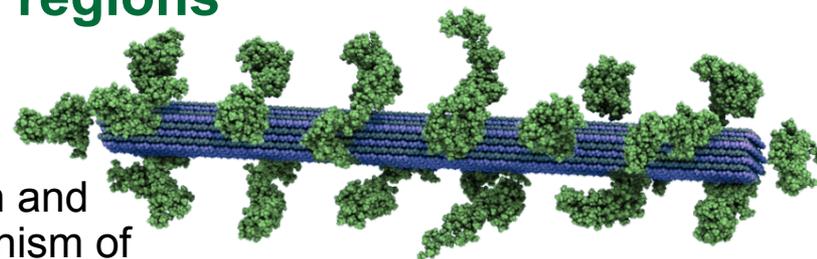
• Biofuels SFA

- HPC simulation of lignin aggregation on cellulose shows stronger binding to crystalline regions



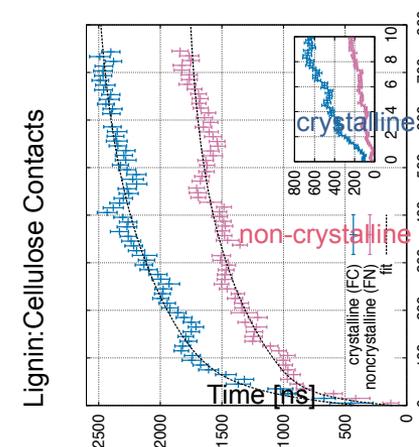
Objective:

- Use of simulations to analyze the interaction of lignin and cellulose at the molecular level to understand mechanism of lignin in recalcitrance. Petascale computer simulations of lignin with cellulose molecules were run on the ORNL Jaguar supercomputer under INCITE award.



New Science:

- Lignin was found to strongly associate with itself and cellulose.
- Non-crystalline regions of cellulose were observed to have a lower tendency to associate with lignin than crystalline regions due to higher hydration.



Top: Molecular model of 52 lignin molecules (green) surrounding a crystalline cellulose fiber (blue)

Bottom: Number of contacts between cellulose and lignin as a function of simulation time.

The increasing contacts demonstrate lignin association with cellulose. The crystalline cellulose (blue) associates more with lignin than non-crystalline (pink).

Significance:

- The results suggest that the recalcitrance of crystalline cellulose to hydrolysis arises not only from the inaccessibility of inner fibers but also due to the promotion of lignin adhesion.

• Lindner, et al. “Solvent-Driven Preferential Association of Lignin with Regions of Crystalline Cellulose in Multimillion Atom Molecular Dynamics Simulation. *Biomacromolecules* (in revision, 2013).

HPC simulation of lignin aggregation on cellulose shows stronger binding to crystalline regions

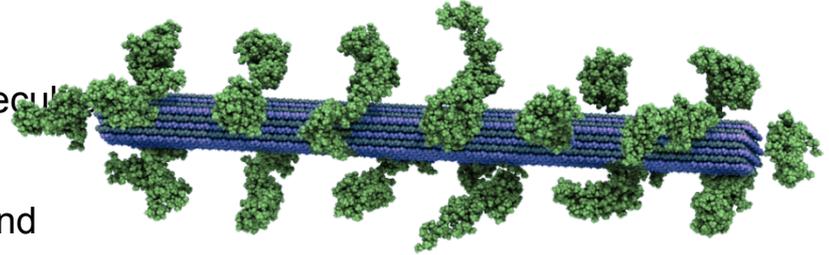
Background:

- Lignin aggregation on cellulose is a major barrier to viable biofuel production.



Approach:

- Petascale computer simulations of lignin with cellulose molecules were run on ORNL's Jaguar supercomputer under INCITE award.
- Two types of cellulose models were simulated: crystalline and non-crystalline.

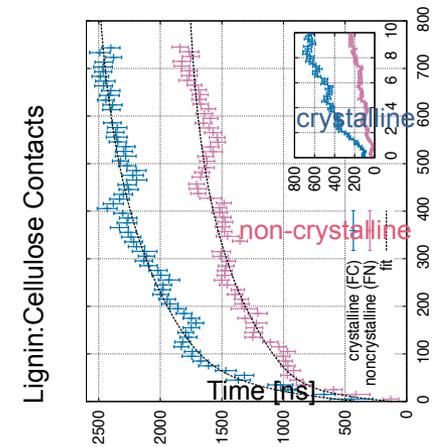


Objective:

- Use of simulations to analyze the interaction of lignin and cellulose at the molecular level to understand mechanism of lignin in recalcitrance.

Results:

- Lignin was found to strongly associate with itself and cellulose.
- Non-crystalline regions of cellulose were observed to have a lower tendency to associate with lignin than crystalline regions.
- This was found to arise from more favorable hydration of the non-crystalline regions.



Top: Molecular model of 52 lignin molecules (green) surrounding a crystalline cellulose fiber (blue)

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Significance:

- The results suggest that the recalcitrance of crystalline cellulose to hydrolysis arises not only from the inaccessibility of inner fibers but also due to the promotion of lignin adhesion.

Gratton, D., Linner, L., Petridis, R., Schulz, J.C., Smith, L. Solvent-Driven Preferential Association of Lignin with Regions of Crystalline Cellulose in a Multimillion Atom Molecular Dynamics Simulation". *Biomacromolecules* (in revision, 2013). Contact: smithjc@ornl.gov