

Molecular principles revealed for cosolvent depolymerization of biomass

Objective:

- Novel biomass pretreatment methods utilizing multifunctional cosolvents, such as tetrahydrofuran (THF) and water, have demonstrated unique functionalities in promoting both biomass solubilization and lignin fractionation.

Approach:

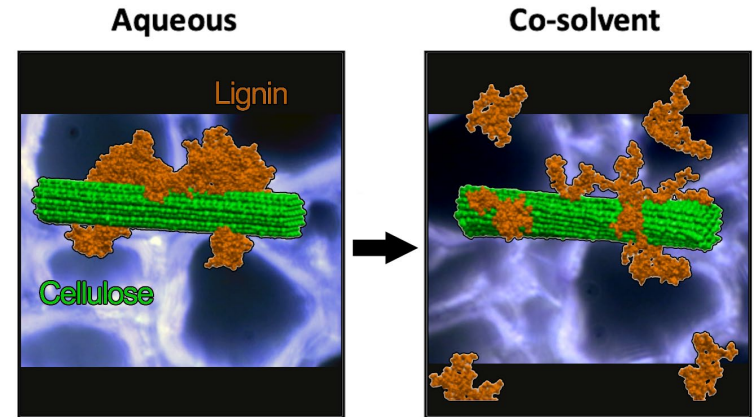
- A multi-scale approach combining molecular dynamic (MD) simulations with nano-scale imaging, and experimental validation was performed to understand cosolvent effects.

Results:

- In the THF cosolvent environment, almost all lignin molecules have dissociated from the cellulose fiber and from each other, changing their structure from compact to extended coil states.
- This exposes inter-unit linkages, rendering them susceptible to acid-catalyzed fragmentation by cleavage of aryl-ether bonds. This also allows better enzymatic access to the cellulose fibers.
- Nanoscale infrared sensors confirm cosolvent mediated molecular rearrangement of lignin in the cell wall of micron-thick hardwood slices and track the disappearance of lignin.
- At bulk scale, dilute acid pretreatment of biomass in a cosolvent mixture liberates hemicellulose and depolymerized lignin from cellulose, allowing unfettered access of cellulolytic enzymes that sustain high rates of cellulose hydrolysis to glucose without enzyme deactivation. expanded state.

Significance:

- The molecular driving forces have been determined behind maximizing total utilization of biomass by simultaneously enhancing both the efficient hydrolysis of polysaccharides and the extraction and depolymerization of lignin. The methodology used is of general applicability in pretreatment science, a critical step towards the rational design and optimization of cosolvent driven biomass deconstruction technologies.



Molecular dynamics models of lignocellulose in aqueous solution (left) and cosolvent mixture (right). The cellulose fiber is shown in green and the lignin molecules in brown. Corresponding images of a single micron-thick poplar slice shown in background.