

# Molecular Driving Forces in Lignocellulosic Biomass Deconstruction

## Objective:

- Summarize and contextualize research aimed at elucidating the molecular-level physical phenomena that drive biomass assembly and deconstruction.

## Approach:

- Review work on the physicochemical forces that keep biomass together *in vivo* and deconstruct it during pretreatment.

## Results:

- Critical processes have been found to be driven by solvation thermodynamics. Water entropy plays a major role.
- Solvent “quality” is key to biomass solubilization and fractionation.
- Amphiphilic effects have recently come to the fore.

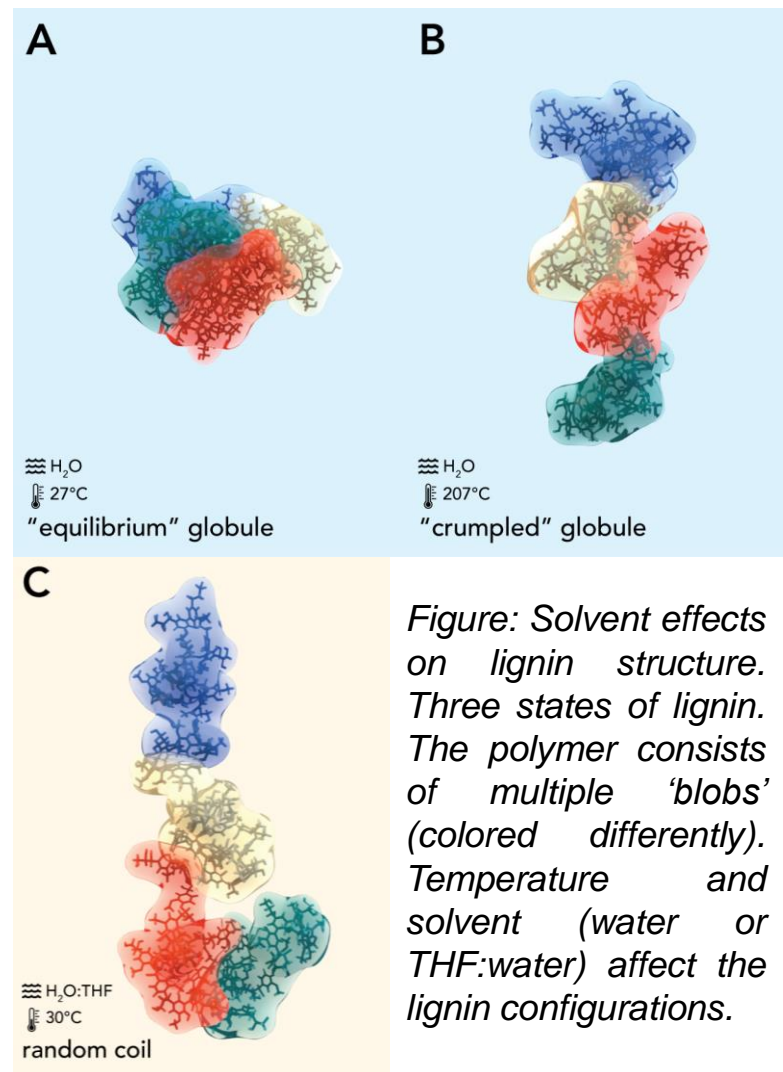
## Significance:

- Molecular driving forces have been determined that stabilize native biomass structures and govern thermochemical pretreatments.
- This understanding can be used in the design of advanced methods for efficiently deconstructing biomass for biofuels and other bioproducts

## BER Biofuels SFA at ORNL

### (Dynamic Visualization of Lignocellulose degradation ...)

L. Petridis & J.C. Smith. “Molecular-Level Driving Forces in Lignocellulosic Biomass Deconstruction.” *Nat. Rev. Chem.* 2018, DOI: 10.1038/s41570-018-0050-6



*Figure: Solvent effects on lignin structure. Three states of lignin. The polymer consists of multiple ‘blobs’ (colored differently). Temperature and solvent (water or THF:water) affect the lignin configurations.*