Mechansims of the Lignin Glass Transition Revealed

Objective:

- Lignin is typically heated above its glass transition temperature to facilitate its industrial processing.
- We characterized the atomic motions giving rise to the lignin glass transition and how they differ above and below the glass transition temperature, T_g.

Approach:

- Molecular dynamics simulations and polymer theory.

Results:

- Below T_g, lignin exhibits mainly internal and localized motions. Above T_g, segmental motions dominate and lead to enhanced chain mobility.
- The segments whose mobility is enhanced above Tg consist of 3-5 lignin monomeric units.
- The temperature dependence of the lignin relaxation time was found to switch from Arrhenius to non-Arrhenius as the temperature is increased above T_g.

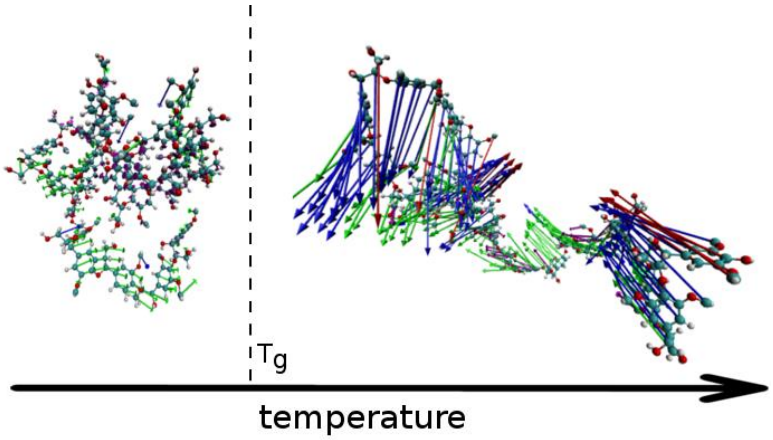

Figure: The motions of atoms in a lignin macromolecule at (left) 25°C and (right) 200°C. The mobility of 3-5 monomer segments is significantly enhanced above Tg. Red arrows represent the largest contribution to the motions, blue moderate and green the lowest

Significance:

- We have characterized the atomic motions that lead to the industrially-important lignin softening above T_g
- Despite the heterogeneous and complex structure of lignin, its glass transition dynamics can be described by concepts developed for chemically homogeneous polymers.

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(Dynamic Visualization of Lignocellulose degradation …)

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