# Catalytic Pulping of Wood

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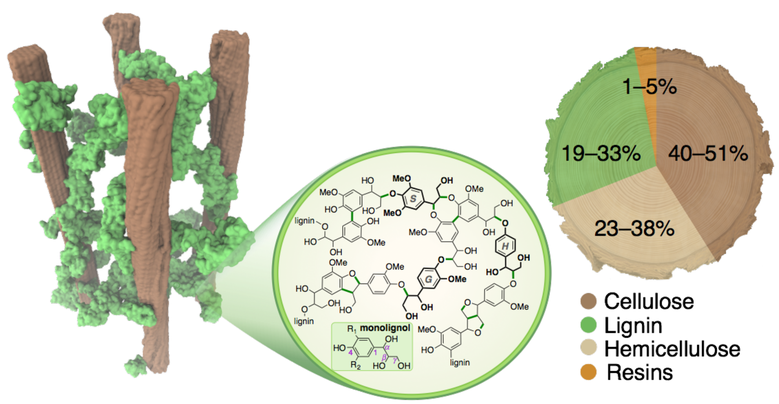
## Need

One of the most energy-intensive steps in the manufacture of the pulp, paper and forest bioproducts is the removal of lignin from biomass.

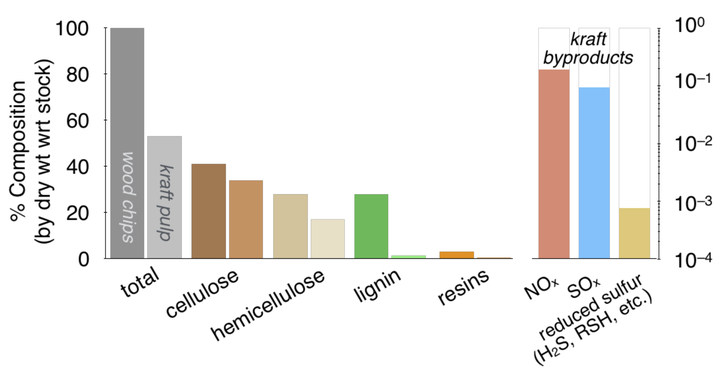
**Biomass at the Molecular Scale**




**The polysaccharides, cellulose (brown) and hemicellulose (tan), are the primary components of plant cell walls. Extensive cross-linking by the phenolic polymer lignin (green) imparts structural rigidity.**

In kraft delignification, wood chips are impregnated with a hot, caustic solution. Polysaccharide deterioration and malodorous compounds are undesired byproducts.

**Effects of Kraft Treatment on Biomass Composition**



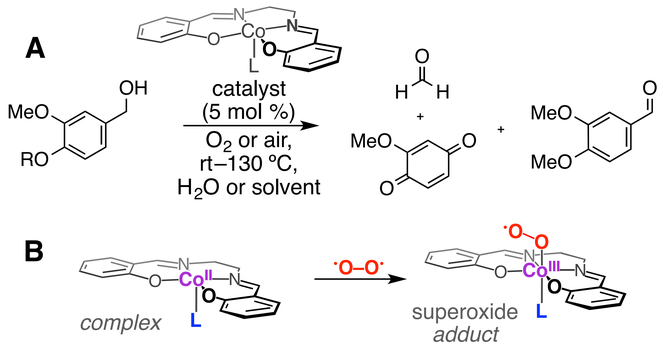

**Treatment of birch chips leads to extensive delignification, but also some degradation of the polysaccharide material. Byproducts include pollutants like NOx, SOx, and malodorous, reduced sulfur species.**

## Approach

Cobalt-based oxidative catalysis offers a promising alternative to kraft treatment.

- Cost-effective due to high natural abundance of Co metal and $O_2$.
- Operation under mild conditions.
- Facile ligand synthesis from inexpensive precursors.

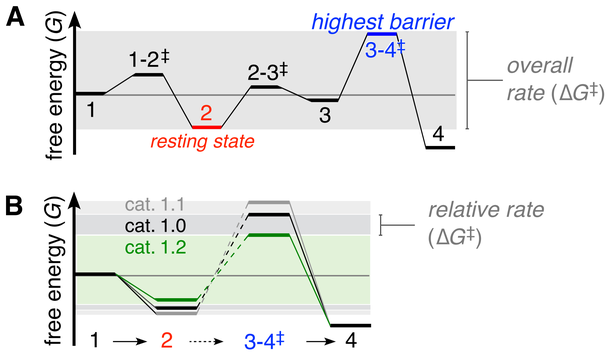
**Cobalt-Catalyzed Delignification**




**A) Initial success in the oxidation of small lignin model compounds. B) Exposing the catalyst to molecular oxygen generates the reactive cobalt-superoxide adduct.**

Computational investigation of the catalytic mechanism provides detailed insight into the chemical factors governing reactivity.

**Predicting Catalytic Efficiency with Computations**

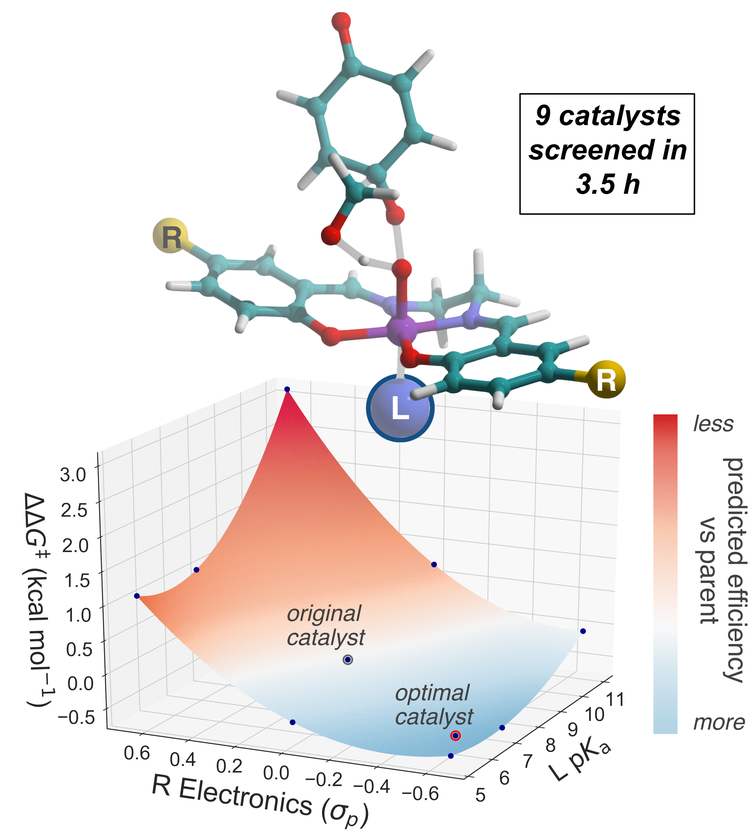



**Overall (A) and relative (B) efficiencies of potential catalysts can be directly estimated from their free energy profiles.**

## Approach (Continued)

By establishing quantitative structure-property relationships (QSPR) between potential and existing catalysts, new leads can be rapidly screened and optimized *in silico*.

**Catalyst Screening and Optimization**




**The catalyst chemical space is rapidly explored for new hits using multivariate QSPR analysis.**

## Benefits

- Odorless, milder process
- increased energy and cost efficiency
- potential pathways to new bio-based products

AGENDA 2020 TECHNOLOGY ALLIANCE

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