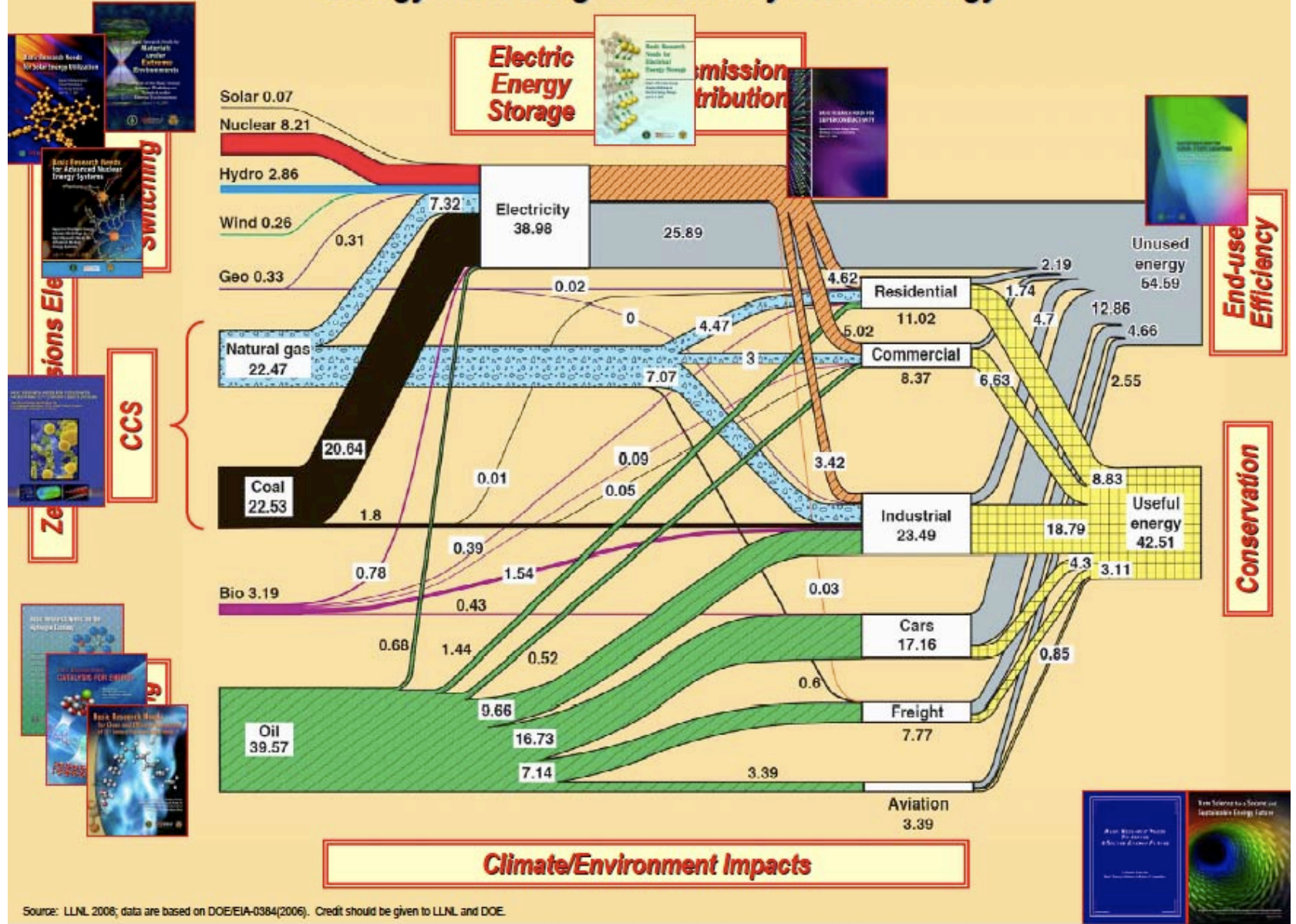
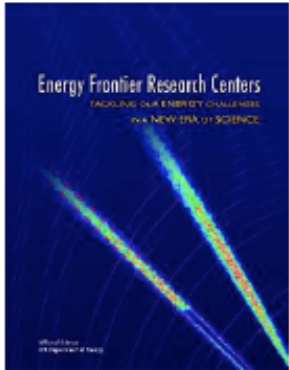


Energy supply and use in the United States

Energy Flow Diagram and Key R&D Strategy





“To harness the most basic and advanced discovery research in a concerted effort to establish the scientific foundation for a fundamentally new U.S. energy economy. The outcome will decisively enhance U.S. energy security and protect the global environment in the century ahead.”

Key characteristics:

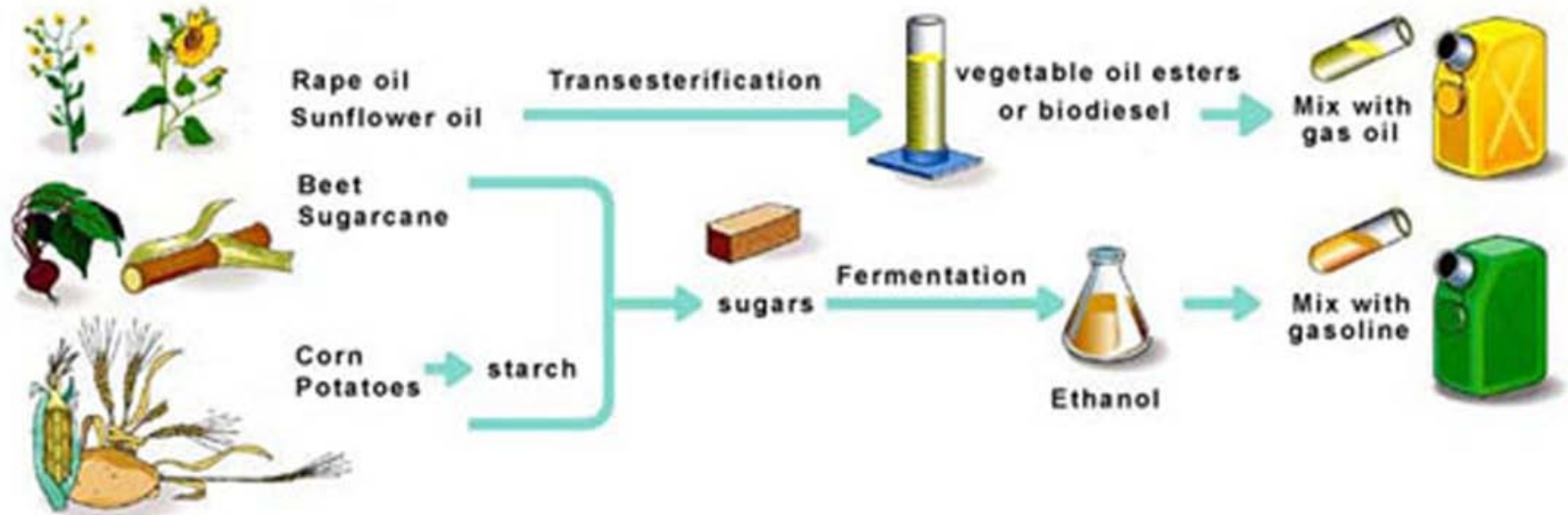
- To engage the talents of the nation’s researchers for the broad energy sciences
- To accelerate the scientific breakthroughs needed to create advanced energy technologies for the 21st century
- To pursue the fundamental understanding necessary to meet the global need for abundant, clean, and economical energy

Be Bold, Imaginative, and Impactful!



**Center for direct catalytic conversion
of biomass to biofuels (C3Bio)**

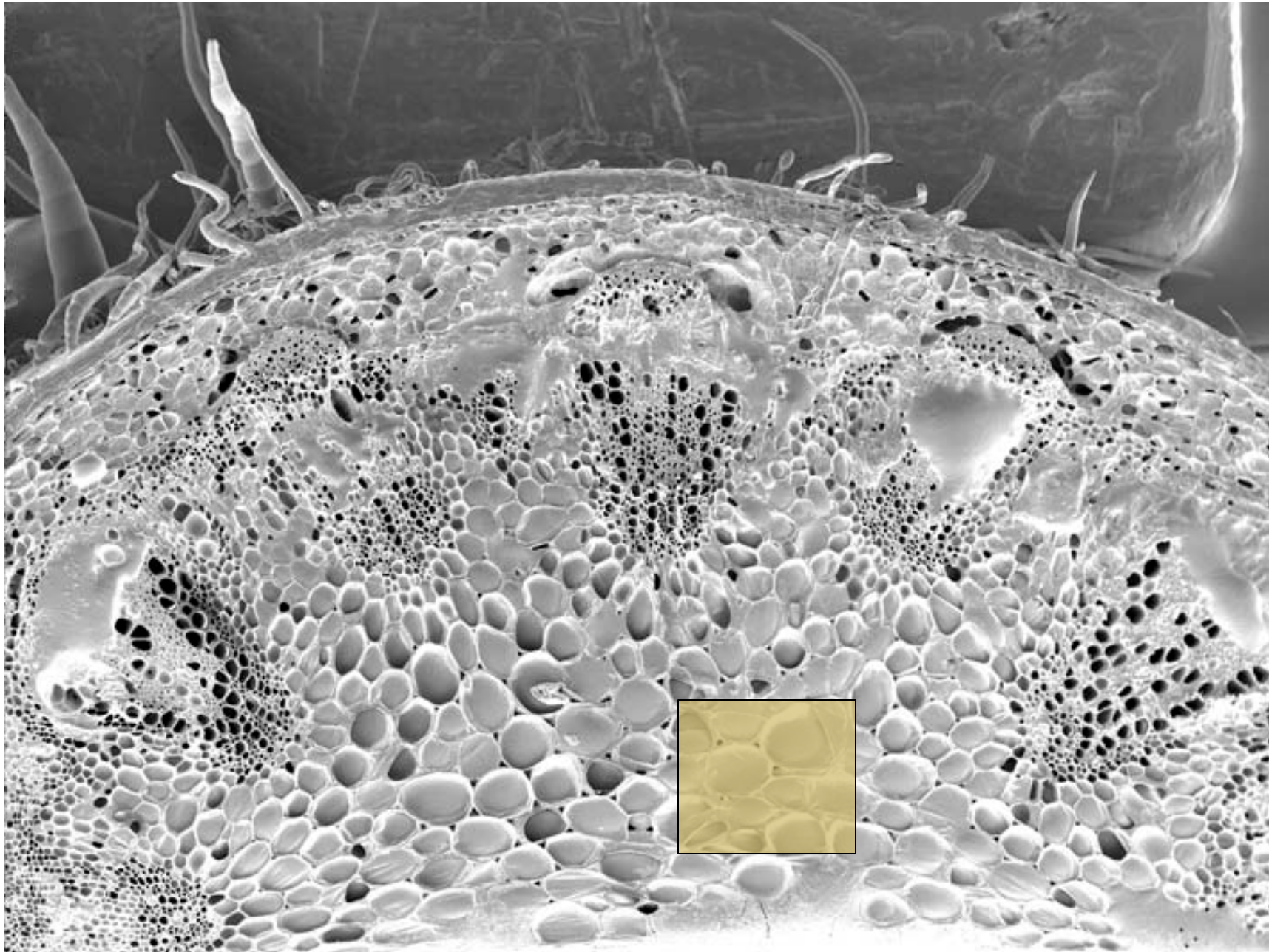
First generation biofuels are derived from starch, sugar or oils



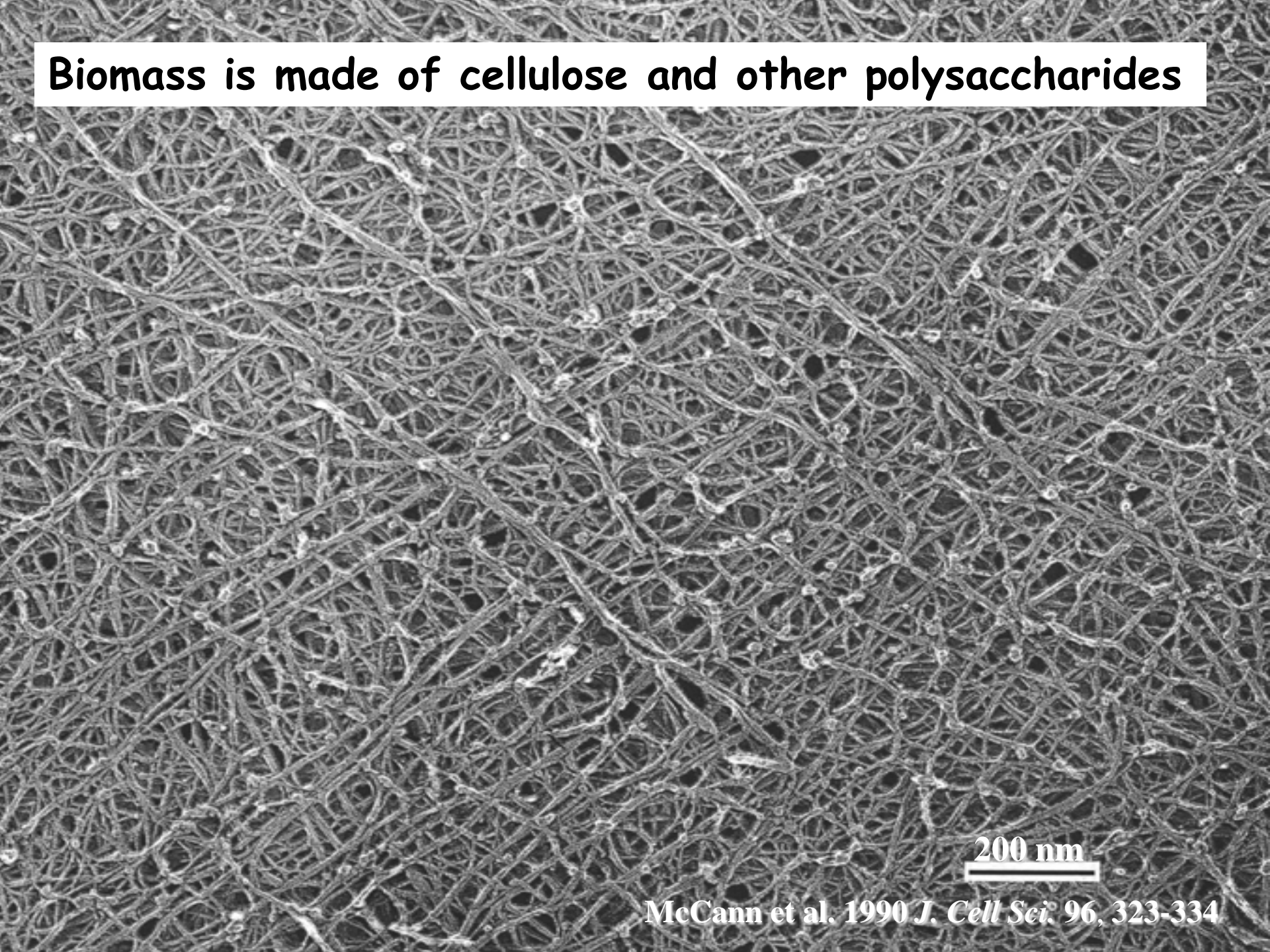
Second generation biofuels... from lignocellulosic biomass



Wilfred Vermerris

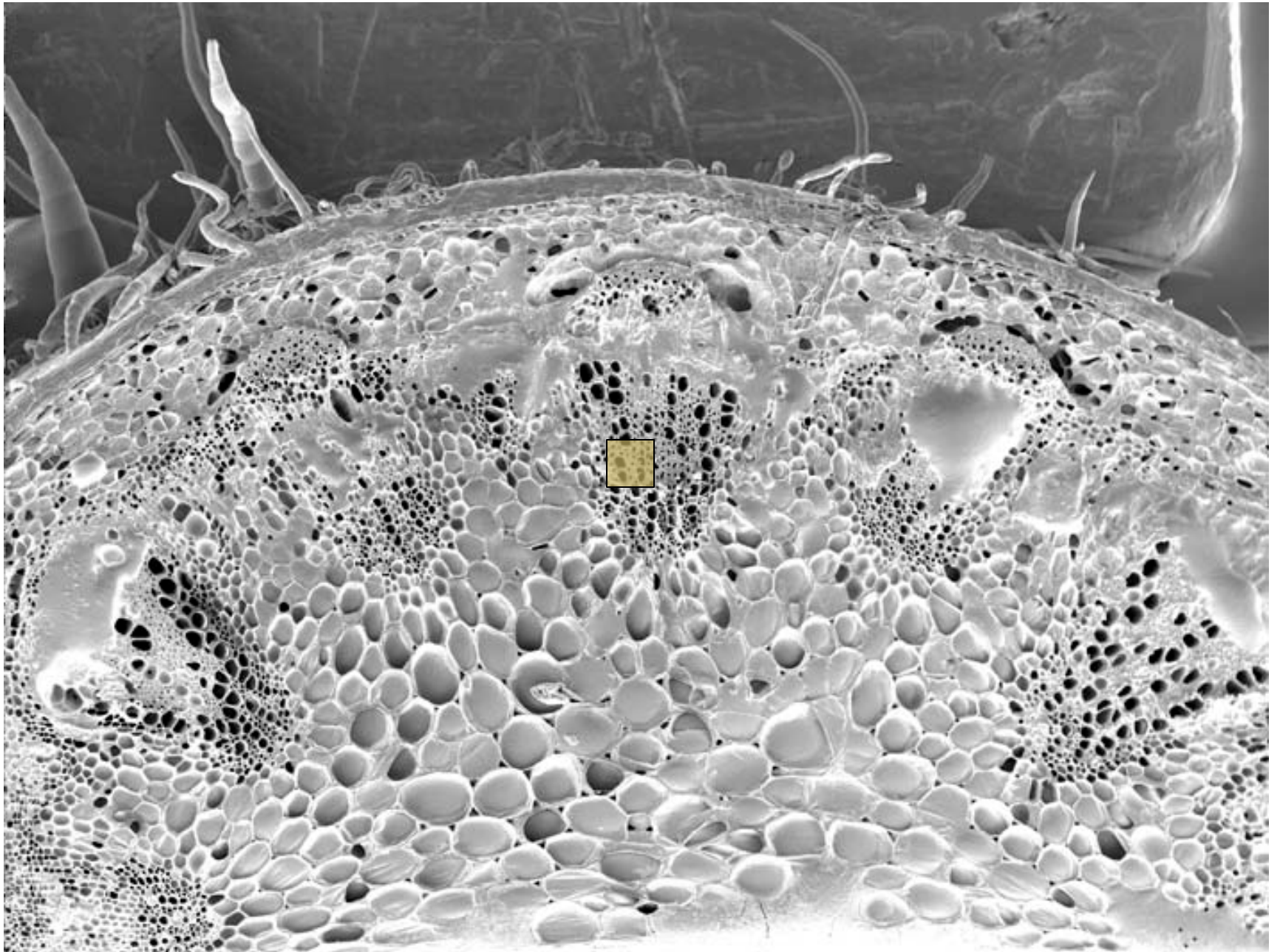


Biomass is made of cellulose and other polysaccharides

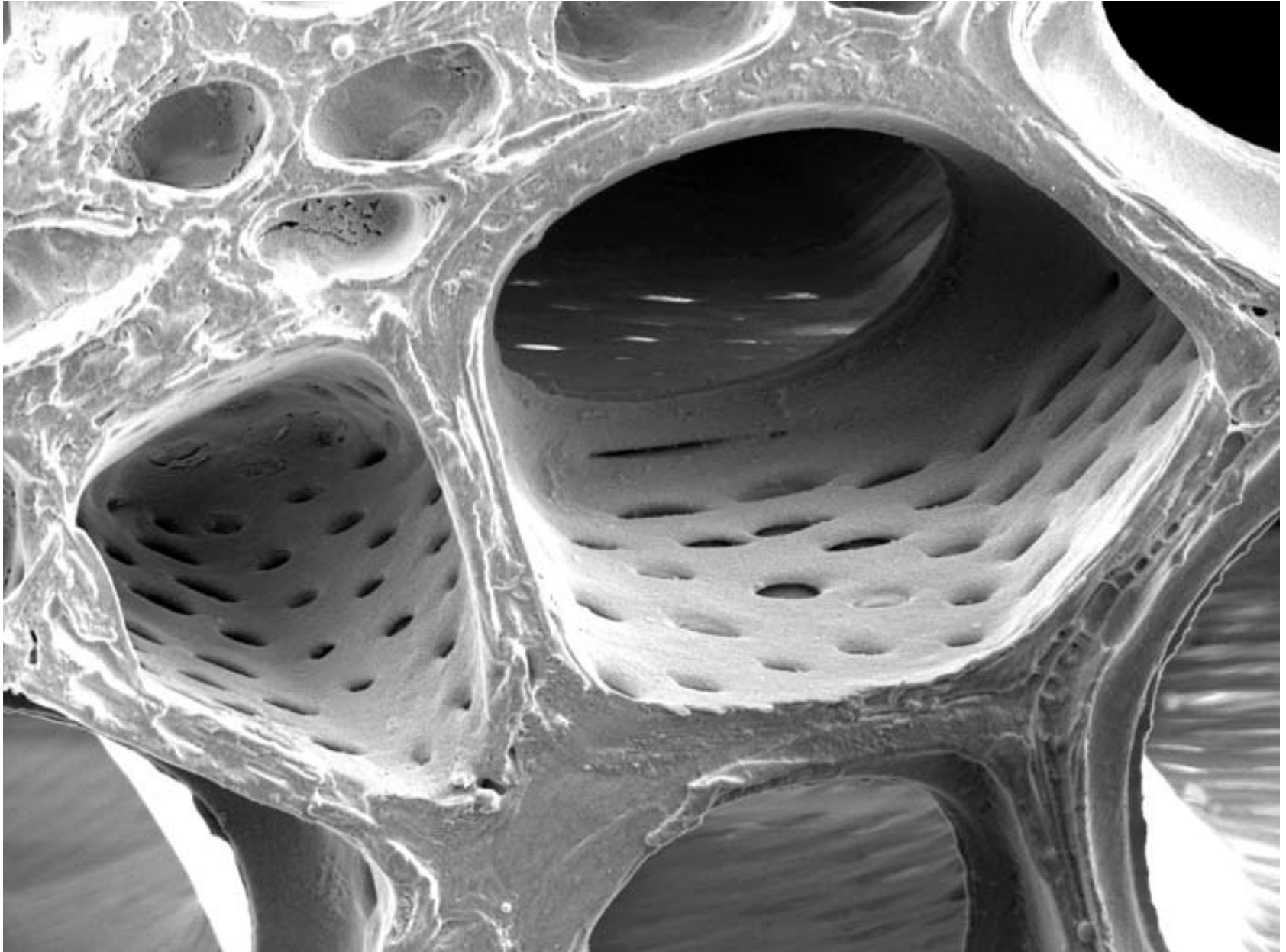


200 nm

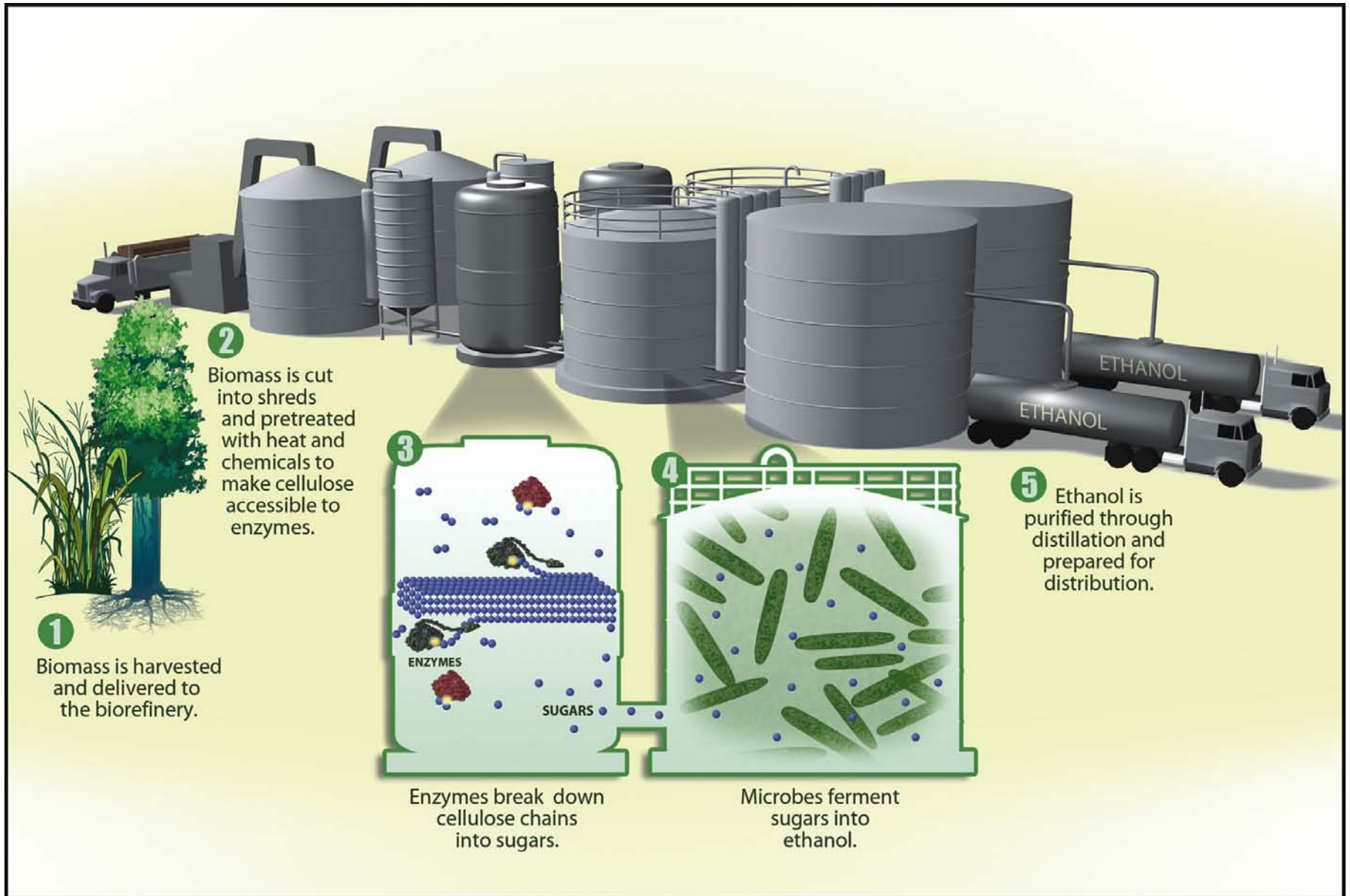
McCann et al. 1990 *J. Cell Sci.* 96, 323-334



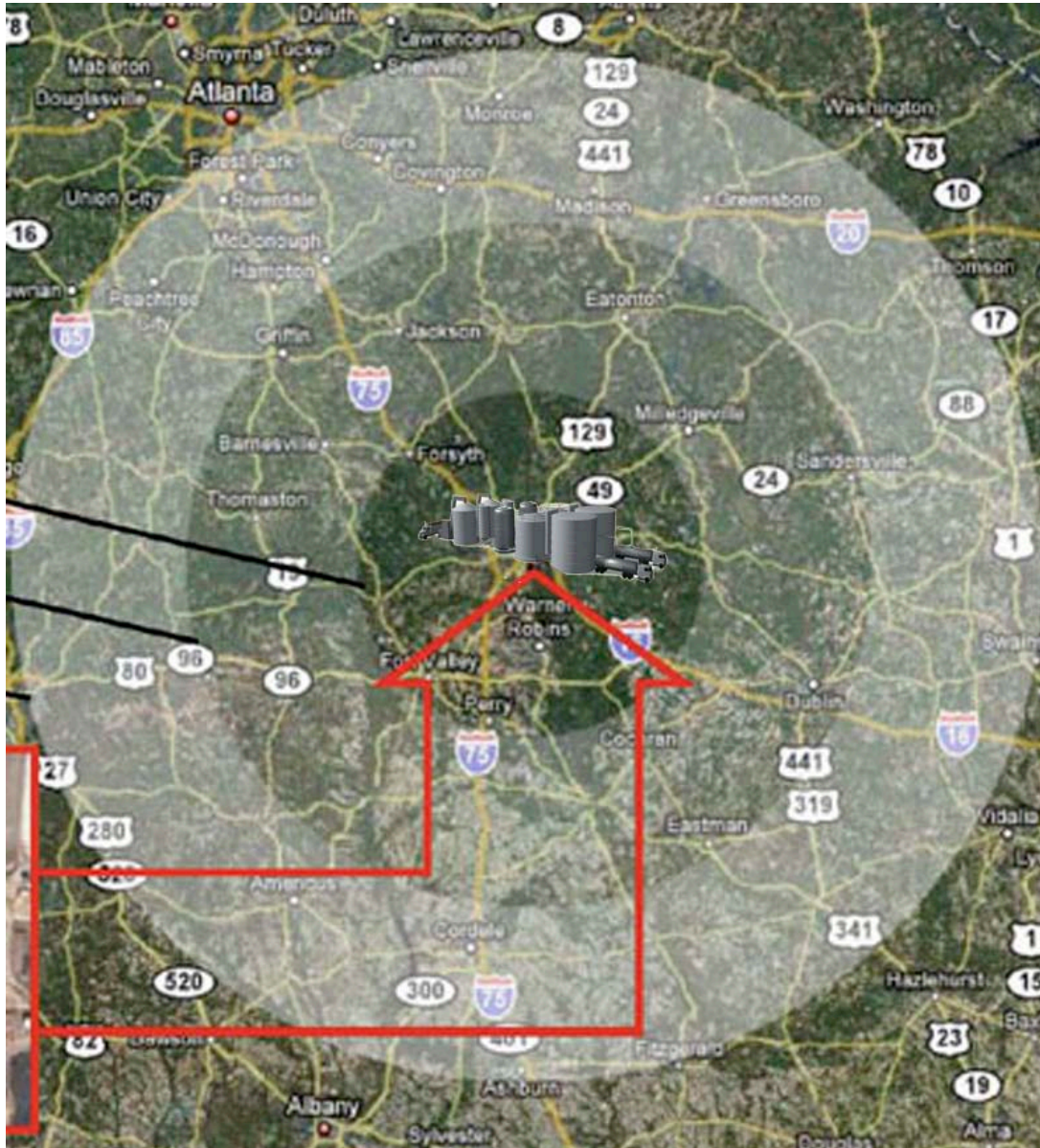
Lignified secondary walls surround some specialized cell types but contribute greatly to the biomass



Biological conversion route for biomass to biofuel



Transport costs will limit where biomass feedstocks are grown



The genetic diversity of maize is estimated at nearly 1.9%

Maize has quality traits for advances in not only grain yield but also biomass and sugar accumulation



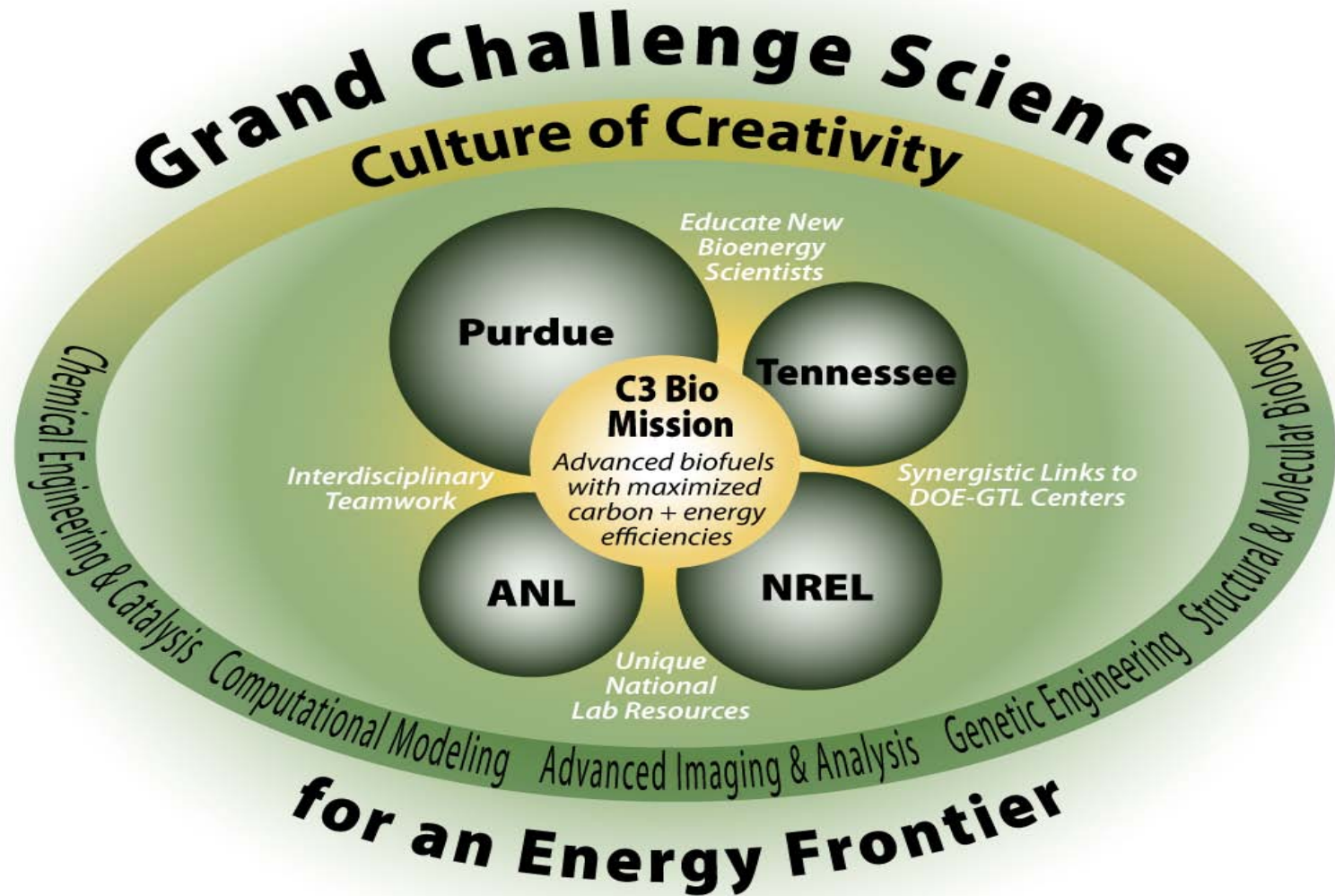
Biomass
Sugar



Grain
Yield



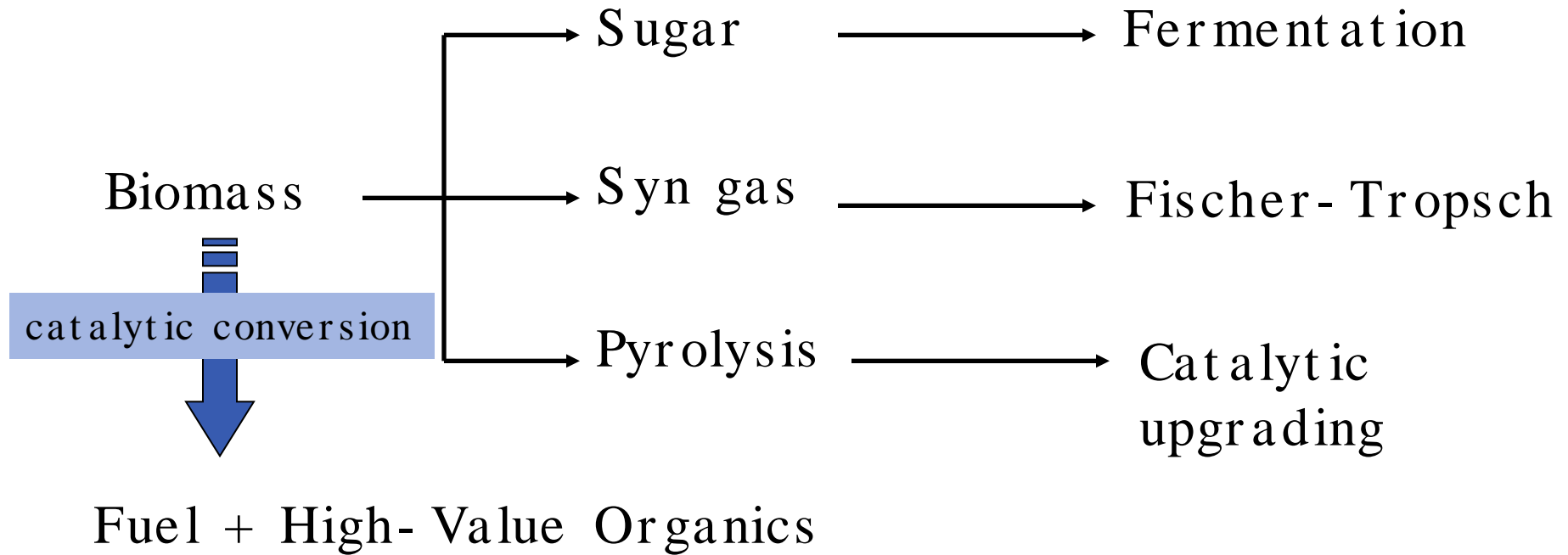
We need to increase dramatically the carbon and energy efficiencies of biofuels production



Desired characteristics of a winning conversion process

- the process is independent of the feedstock species
- it will maximize the carbon and energy conversion efficiency (amount of product recovered per unit biomass)
- desired co-product streams can be recovered
- can be scaled to smaller, even mobile, biorefineries

Conversion technologies for next-generation biofuels



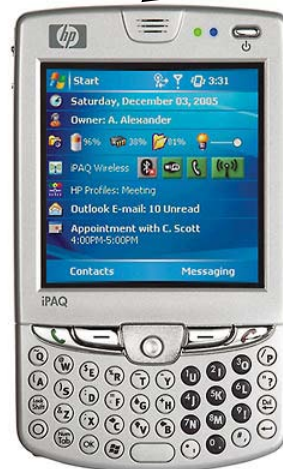
The petrochemical industry: a 20th century success story built on chemical catalysis



drop-in biofuel



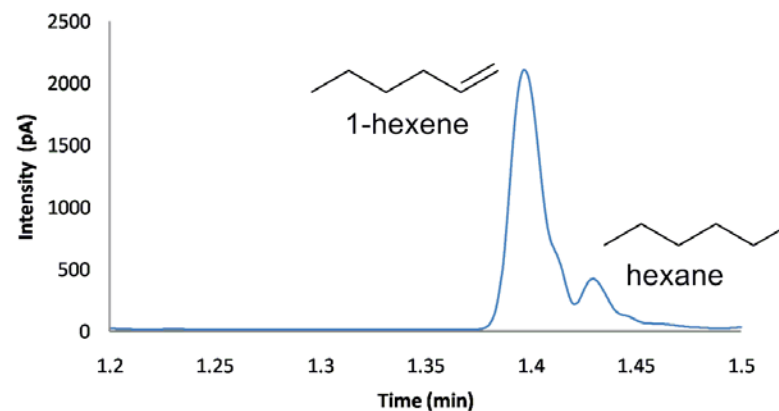
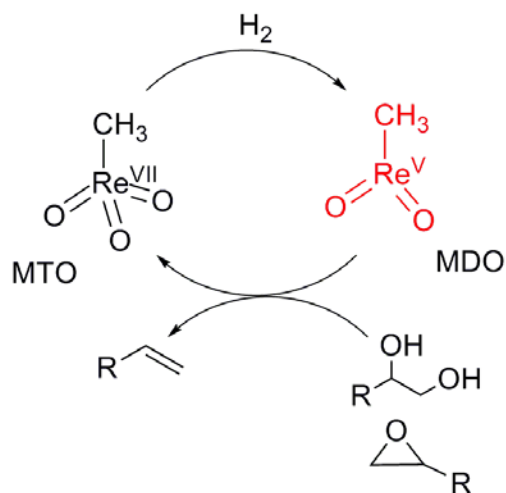
Interesting Materials



Magnificent six - the six chemicals used as starting materials in the petrochemical industry

Converting sugars to alkenes: diol- to- alkene reaction

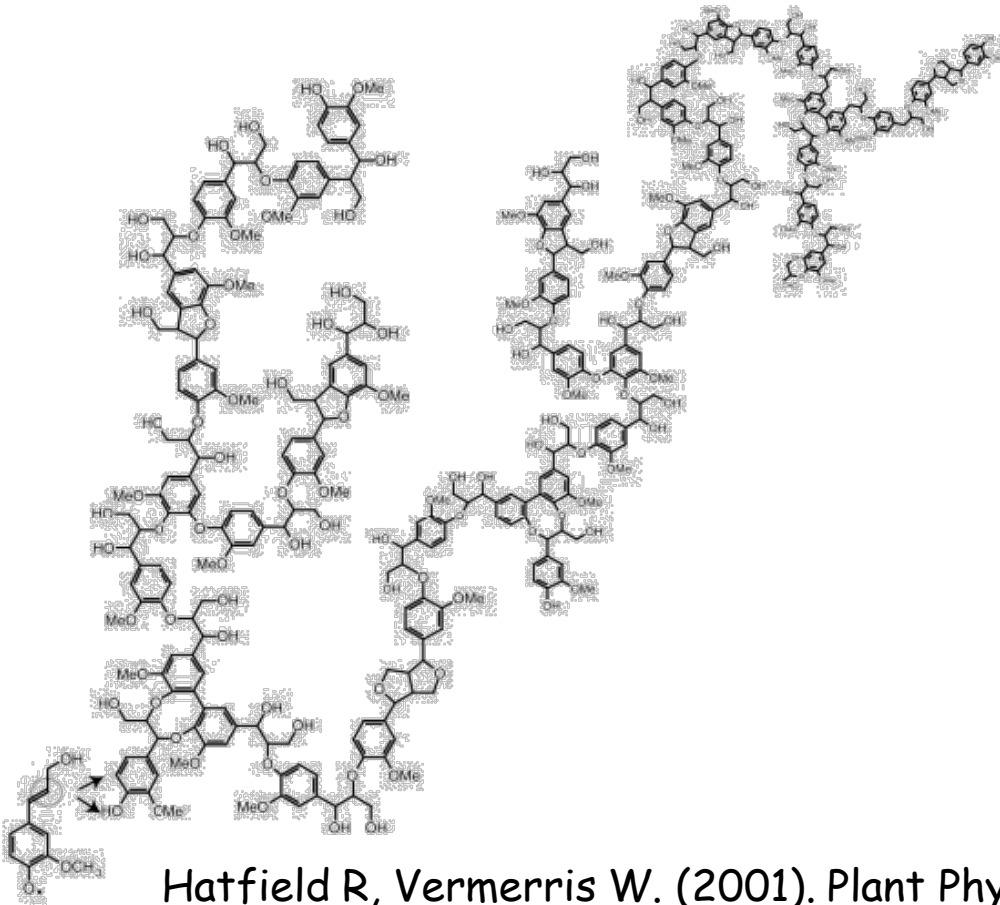
Mechanism



J. E. Ziegler, M. J. Zdilla, A. J. Evans, and M. M. Abu-Omar, "H₂-Driven Deoxygenation of Epoxides and Diols to Alkenes Catalyzed by Methyltrioxorhenium" *Inorg. Chem.* **2009**, 48

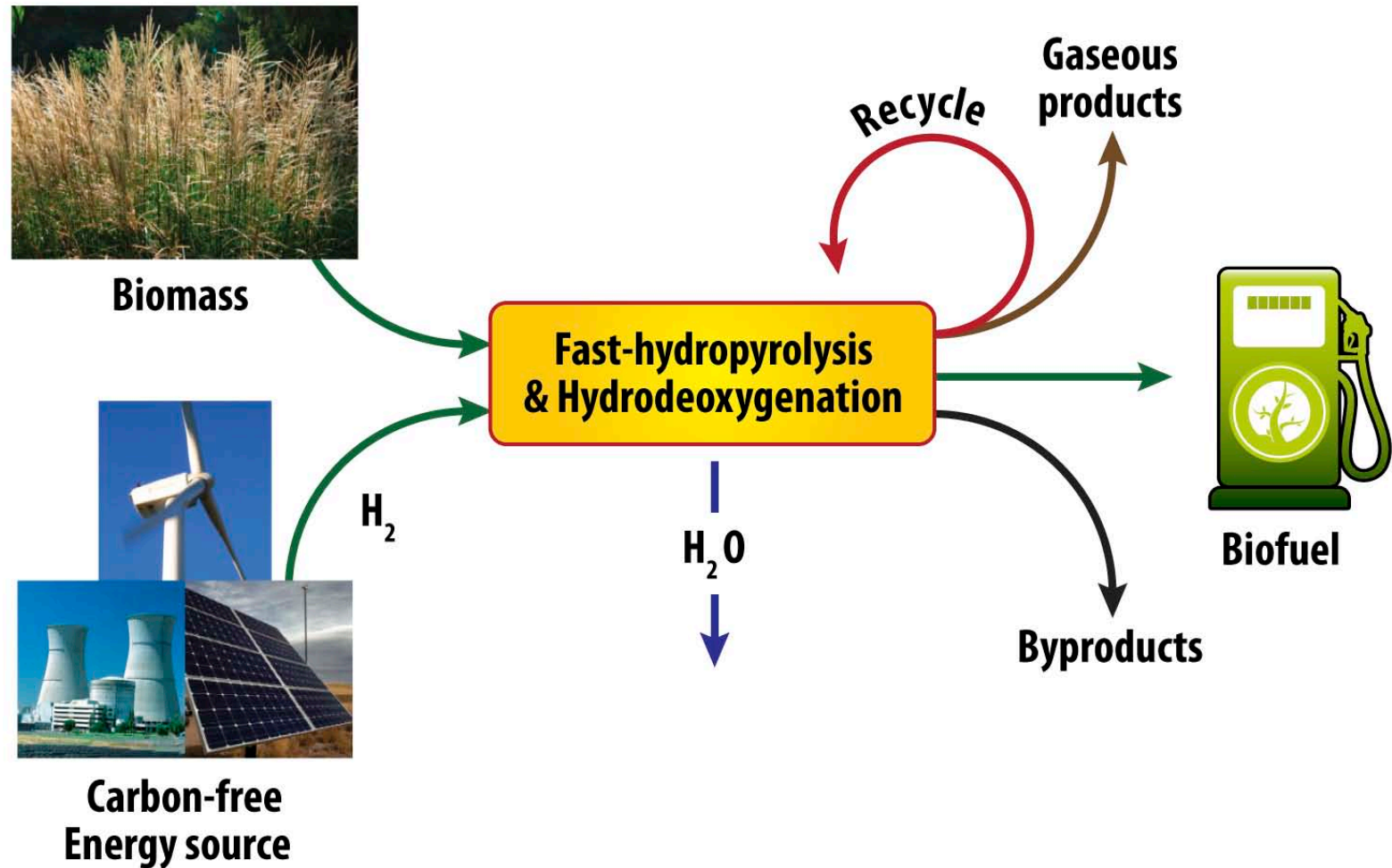
Lignin is an opportunity as well as a challenge

- UV resistance
- structural support
- water transport

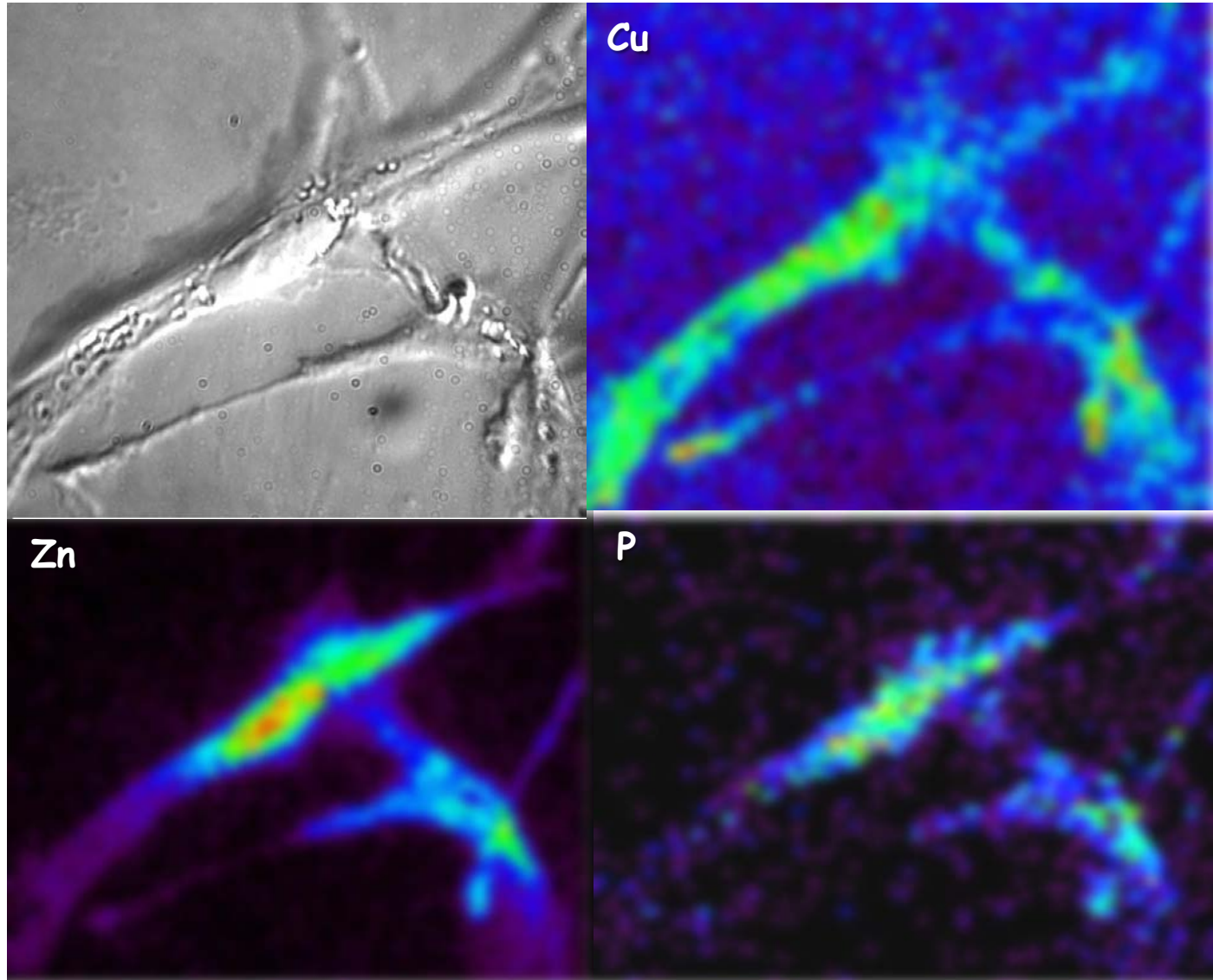


Hatfield R, Vermerris W. (2001). *Plant Physiol.* 126: 1351-1357

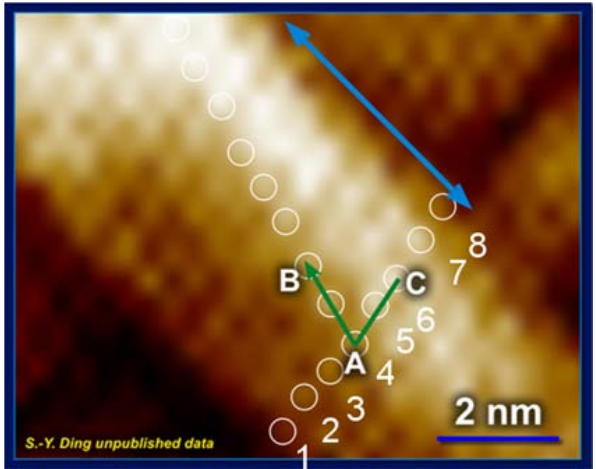
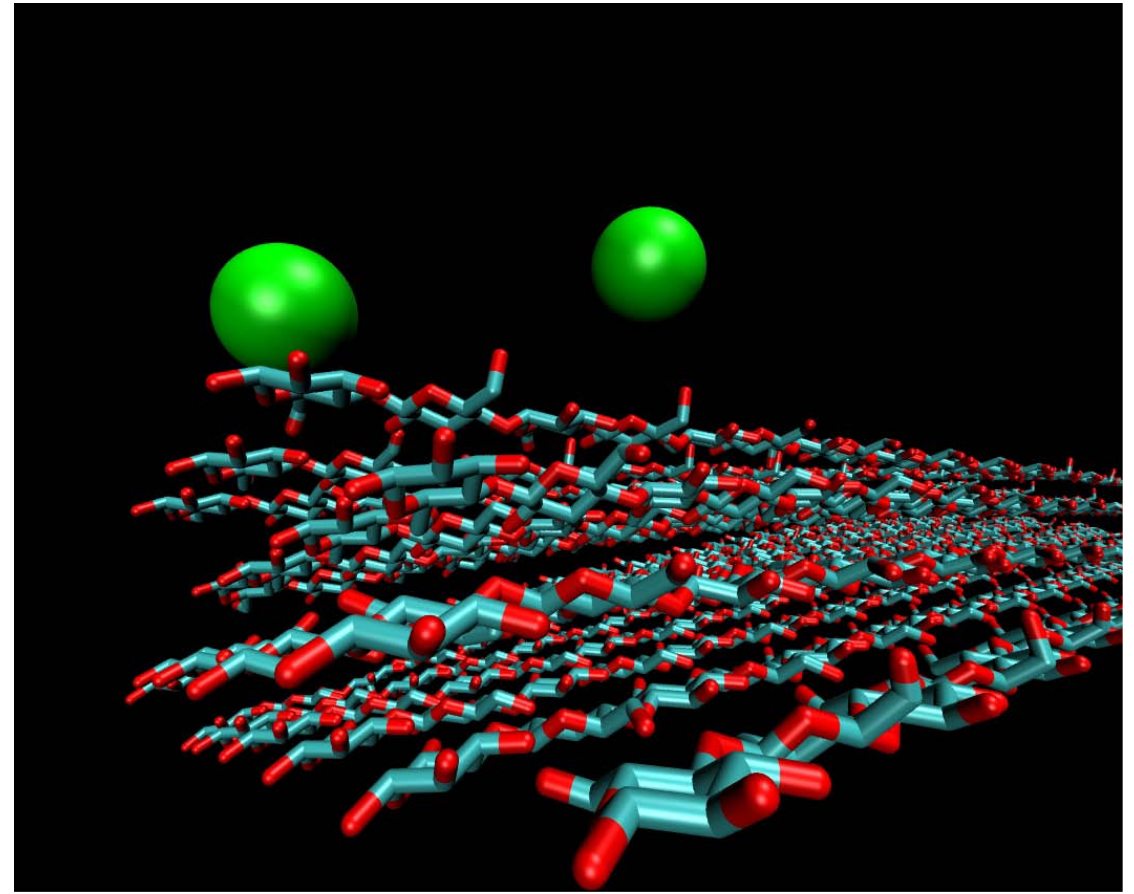
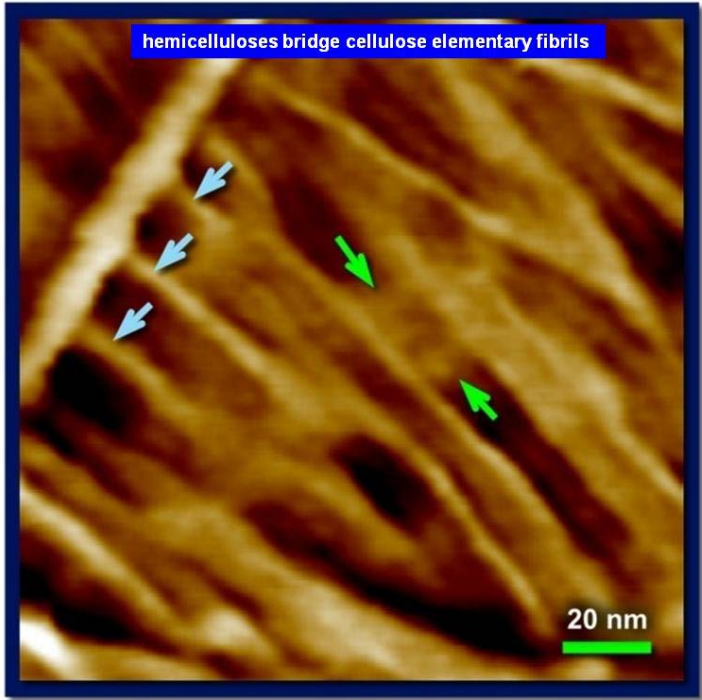
High-temperature treatments may produce a bio-crude oil for biorefinery fractionation



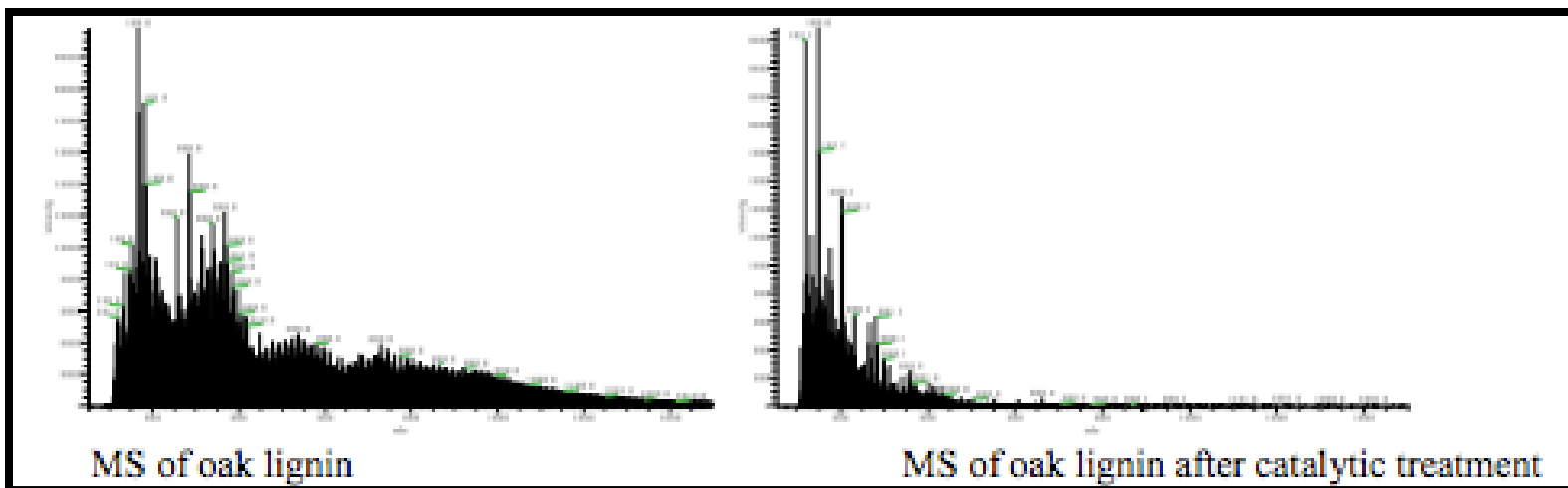
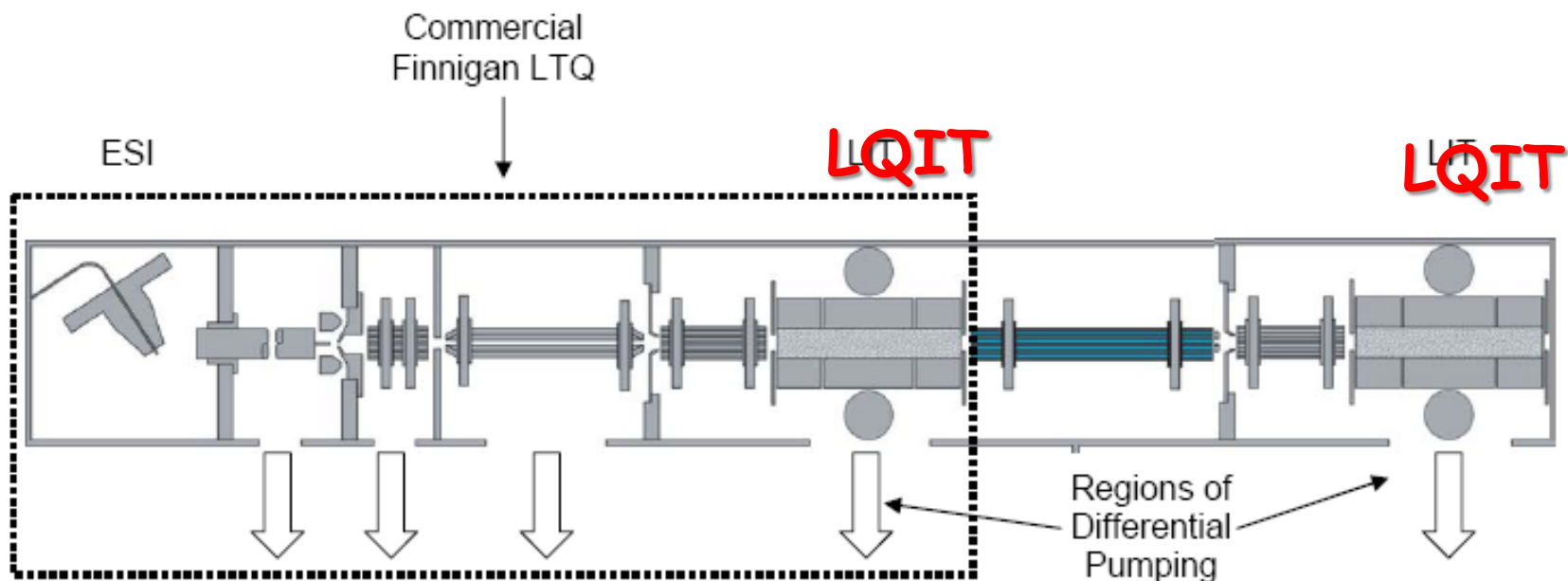
X-ray fluorescence imaging - capable of mapping distribution of metals in complex tissues with $0.5 > 0.1$ micron resolution



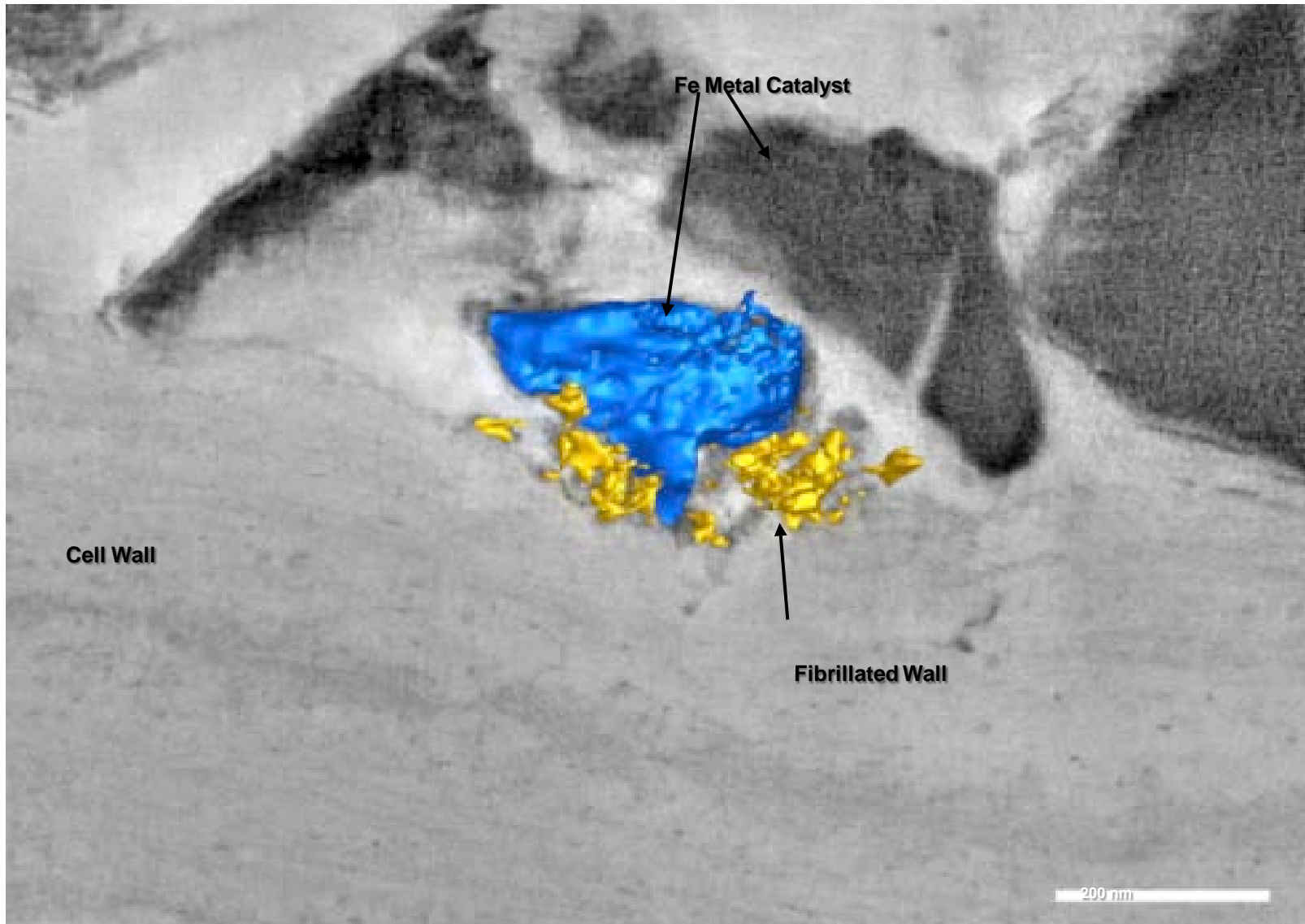
Imaging and modeling of cellulose microfibrils and metal catalysts



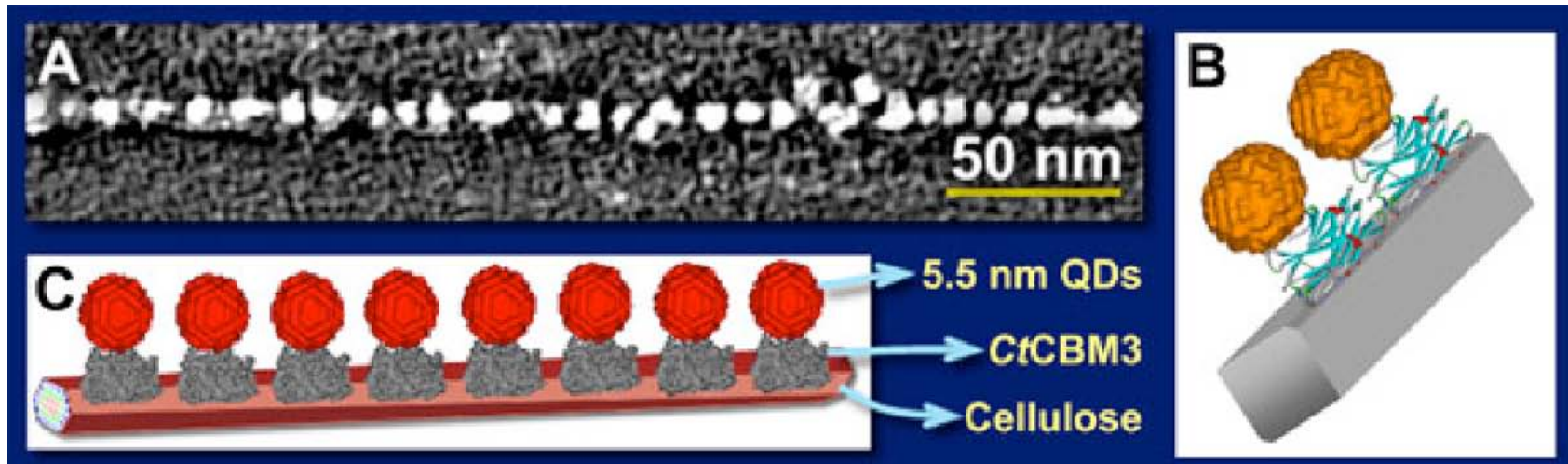
A new tandem-linear quadrupole ion trap (TWIN) to analyze highly complex mixtures of reaction products in MS^n experiments



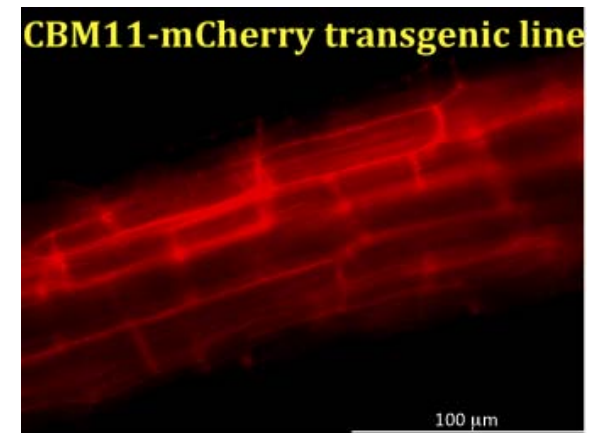
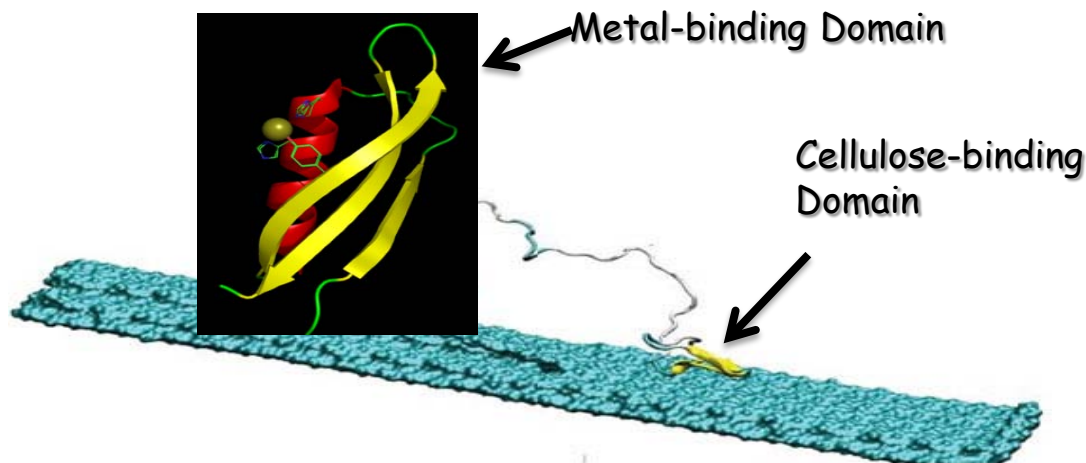
A metal catalyst contacts a very limited surface of cell wall.
Can we deliver metal catalysts throughout the volume of the cell wall and target them to specific molecules?



Tailored biomass - introducing catalysts and catalytic sites as plants grow



Quantum dots are specifically labeled on the planar face of crystalline cellulose directed by carbohydrate-binding module (CBM).



Long-term impacts of success

- *more than double* the carbon captured into fuel molecules compared to biological catalytic routes;
- *expand* the product range to alkanes and new energy-rich aromatic liquid fuels and other value-added molecules currently made through oxygenation of petrochemicals;
- *retain* the current liquid fuel infrastructure;
- *enable* the utilization of engineered energy crops;
- *minimize* the agricultural footprint through scalable and distributive hydrocarbon refineries that substitute for the present-day oil refinery.





Purdue University: M. McCann (Director), M. Abu-Omar (Associate Director), R. Agrawal, N. Carpita, C. Chapple, K. Clase, N. Delgass, H. Kenttämä, N. Mosier, F. Ribeiro, G. Simpson, C. Staiger, D. Szymanski, K. Thomson

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Argonne National Laboratory: L. Makowski, J. Lal

University of Tennessee: J. Bozell, C. Barnes, A. Buchan

