Center for Direct Catalytic Conversion of Biomass to Biofuels (C3Bio)
EFRC Director: Maureen McCann
Lead Institution: Purdue University

Mission Statement*: To integrate fundamental knowledge and enable technologies for catalytic conversion of engineered biomass to advanced biofuels and value-added products.*

Transforming Biomass Utilization for Advanced "Drop-in" Biofuels. Plants fix and chemically reduce carbon dioxide from the atmosphere with high efficiency, using solar energy to construct sugars and aromatic molecules that are stored as lignocellulosic biomass, a renewable resource for domestic energy available from U.S. agriculture and forestry. The major components of biomass are polysaccharides and lignin, the latter accounting for 15 to 25% by weight. Second-generation biofuels are obtained from biomass by using biological catalysis to use the carbon atoms in plant cell wall polysaccharides for the production of ethanol. However, this scenario is both carbon- and energy-inefficient. First, biological conversion routes use only the polysaccharide component of the wall, hydrolyzing polysaccharides to sugars as the carbon source for microbes. Second, the presence of lignin interferes with access of hydrolytic enzymes to polysaccharides, thereby inhibiting their conversion to sugars. Third, only one-third of carbon atoms in the biomass are captured into fuel molecules since living microorganisms required to ferment sugars to biofuels consume some sugars for their own growth and respire carbons as carbon dioxide. Doubling the efficiency would halve the land requirement for growing bioenergy feedstocks. In contrast to biological conversion pathways, the power of chemical catalysis to transform biomass components directly to liquid hydrocarbons and aromatic co-products (third-generation biofuels) is an underexplored area of science that has tremendous potential impact. Our Center aims to make revolutionary advances in the production efficiencies by which biomass carbon is converted into liquid hydrocarbons and other energy-rich molecules by the rational and synergistic design of thermal and chemical conversion processes and the biomass itself.

Research Goals. Our interdisciplinary research team of biologists, chemists and chemical engineers is organized to address four critical roadblocks, our **core goals**:

Core Goal 1: Adding value to lignin by enabling its catalytic conversion. Lignin is an abundant by-product of biorefinery operations, and comprises 40% of the energy content in biomass, but is not utilized to make high-value fuels and co-products. We address knowledge gaps through oxidative and reductive catalytic chemistry to use lignin as a substrate for the production of useful molecules; the ability to analyze lignin and its reaction products; and determining how lignin content, composition and architecture impact the reaction products of thermal or chemical catalyses.

Core Goal 2: Synthesis, assembly and deconstruction of cellulose microfibrils. The structure of the cellulose microfibril, its size, crystallinity and potential aggregation in macrofibrils in plant cell walls, is a second major factor in the recalcitrance of biomass to deconstruction. There is limited understanding of plant microfibril structure, heterogeneity, biochemical mechanism of synthesis, and integration with other matrix polysaccharides and phenylpropanoids. We develop this fundamental knowledge in order to gain control over microfibril synthesis, structure and properties together with the development of catalytic deoxygenation chemistry and selective bond breaking to enable efficient transformations of polysaccharides into useful products.

Core Goal 3: Engineer tailored biomass for highly efficient, direct catalytic conversion to liquid fuels and value-added products. Understanding the processes of wall assembly in the living cell are important to enable 1) formulation of strategies for deconstruction and 2) incorporation of *Trojan horse* catalysts into the cell wall in living plants. A key aspect of catalyst-substrate interactions is the accessibility of catalysts to the chemical bonds with which they are designed to react. We aim to engineer biomass variants to incorporate catalysts, co-catalysts, or functionalized catalytic sites into cell walls as the plant grows, simplifying reaction steps in subsequent processing and alleviating the biphasic barrier between the catalyst in solution and the solid polymeric biomass.

Core Goal 4: Fast-hydropyrolysis to maximize carbon efficiency. Thermal treatments deconstruct biomass into an array of liquid and gaseous products along with some char. However, the bio-oil from fast-pyrolysis has an extremely high oxygen content (35 to 40% by weight), and its energy content is barely half that of petroleum. Fast-hydropyrolysis has the potential to generate intermediate products for catalytic upgrading from highly recalcitrant biomass components. On a systems engineering level, this maximizes carbon efficiency while minimizing the hydrogen inputs necessary for deoxygenation. We aim to develop a detailed understanding of how fast-hydropyrolysis and *in situ* hydrodeoxygenation in the presence of appropriate catalyst(s) can lead to advanced (drop-in) liquid fuels.

Cross-cutting technology resources. Novel mass spectrometric and spectroscopic technologies are being developed for analysis of the products of catalytic reactions with biomass molecules in real time. Using unique National Lab resources, we also are developing an integrated set of powerful imaging techniques and data visualization models to study biomass-catalyst interactions at resolutions ranging from ~200 nm (light microscopy) to Ångström (X-ray).

The transformational knowledge gained will form the basis for novel catalysts and reaction chemistry for conversion of biomass to advanced liquid fuels and chemical feedstock. The long-range impact of our research mission will be to more than double the carbon captured into fuel from biomass over biological conversion routes, and expand the product range beyond ethanol to alkanes and new energy-rich aromatic liquid fuels that utilize the current liquid fuel infrastructure and to other high-value hydrocarbon products.

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