Center for direct Catalytic Conversion of Biomass to Biofuels (C3Bio)
EFRC Director: Maureen McCann
Lead Institution: Purdue University
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Mission Statement*: To master the ability to reconfigure all partially reduced carbon from plant cell walls into desired molecules.*

New capabilities to predict, design and control the chemistries of carbon could enable the transition from fossil-based to sustainable transportation fuels. Lignocellulosic biomass, a renewable and carbon-neutral resource, has the potential to displace an estimated annual equivalent of three billion barrels of oil in the U.S. alone. However, biomass has only one-third the energy density of crude oil and lacks petroleum's versatility as a feedstock for fuels and chemicals. These limitations keep biomass conversion below the efficiency level needed for strategic impact while the scientific challenge of routing carbon from one molecular context to another remains unmet.

The polysaccharides and lignins of the plant cell wall form a complex, cross-linked polymeric structure of substantial physical and chemical resilience that impedes access of catalysts to targeted chemical bonds. Its complexity results in heterogeneous product streams after catalytic or pyrolytic processing. Cross-links among plant cell wall biopolymers generate nanoscale architectures and distinct mesoscale domains that have dramatically different properties than those observed in mixtures of biopolymers. C3Bio research demonstrated that the disparity between theoretical and actual yields of liquid hydrocarbons and high-value chemicals is a consequence of this structural complexity. C3Bio will now develop critical systems-level understanding of how biomass structural complexity at molecular, nanoscale, and mesoscale levels impacts the yields and selectivities of desired reaction products from catalytic and pyrolytic transformations. We will establish the fundamental science required to modulate cell wall complexity and catalytically transform intact biomass in order to gain unprecedented control of effective routing of carbon: we will specify both the structures within, and the reaction products from, lignocellulosic biomass.

Goal 1: Develop Catalytic and Pyrolytic Processes Specifically Designed for the Structural Complexity of Biomass. We will investigate the kinetics and mechanisms of catalytic and pyrolytic pathways to advance applicability and selectivity in intact biomass conversion and will use native and synthetic biopolymers and biomass genetic variants to define modified substrate performance in conversion pathways. Goal 1 impacts include lignin evolving from a material used primarily as biorefinery process fuel to a material with utility and value equal to that of biorefinery carbohydrates. We will gain ability to deliver intermediate products from biomass polysaccharides in high yields and with carbon atom conservation for upgrading to drop-in liquid fuels. Pyrolysis will become a feasible technology to make simplified bio-oils for HDO catalysis.

Goal 2: Redesign the Structure of Biomass for Carbon- and Energy-efficient Catalytic and Pyrolytic Transformations*.* C3Bio data on biomass performance in catalytic conversion provide new targets for the genetic engineering of tailored biomass, push the state-of-the-art of meso-scale and multi-scale modeling, and allow for greater predictability and understanding of properties of molecular architectures. At mesoscale, we will modulate localized carbon density, cell-cell adhesion, and target modifications to specific cell types. Multi-scale modeling will accelerate identification of the most chemically labile and stable linkages. Goal 2 impacts will be new understanding to use trait stacking to increase the intrinsic carbon density of the biomass and also brittleness at the time of comminution to produce optimized biomass. A codesign approach will maximize yield and selectivity of reaction products by modifying the substrates *in planta* and creating novel catalyst delivery systems.

Goal 3: Deliver Innovative Pathways for Targeted Product Portfolios from Tailored Biomass. Post-catalytic residues provide modified substrates and architectures for subsequent transformations. We will apply our imaging and analytical toolkits to identify the control points and deliver legacy scientific understandings of how chemical reaction kinetics and biomass properties at the nano-scale (porosity, surface chemistry) and meso-scale (particle size and geometry) affect product formation rates and product profiles. We aim to enable advanced catalyst, reactor, and biomass design beyond "no carbon left behind" to achieve unprecedented control over the routing of carbon from biomass into fuels and chemicals – "a place for every carbon and every carbon in its place".

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