Deconstructing Nature's Structural Material for Biofuels

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Abstract
In early February, Environmental Protection Agency announced that it expects the biofuels industry to produce 6.5 million gallons of cellulosic ethanol this year, a fraction of the 100 million gallons anticipated by the Energy Independence and Security Act of 2007 (EISA). Currently, predominant production of biofuel is from corn-based ethanol, but EISA limits the amount of ethanol that may be derived from corn starch and mandates 16 billion gallons of cellulosic ethanol to be blended into the transportation fuels by 2022. The challenges faced by the lignocellulose-to-ethanol conversion technologies are critically linked to the uncertainties of the physical properties of the feedstock. Plant cell walls were constructed by evolution to deal with environmental stress and pathogen attack. The recalcitrant nature of the cell wall can be attributed as one of the major factors responsible for the failure of the cellulosic ethanol industry to even come close to meeting the mandated goals.

We will describe our theoretical approaches to obtain a molecular level understanding of the central problem, how cellulose, an assembly of polymers of glucose, can be effectively isolated and disassembled to its basic building block. We have extended biophysical methods that have been successfully applied to study protein folding/aggregation and biomolecular recognition/binding to characterize the underlying stability of cellulose that comes from the dense hydrogen bonding network constructed among the crystalline-ordered polysaccharide chains. Lignin is the most recalcitrant component of lignocellulose and interferes with enzymatic degradation of cellulose. We have been carrying out computations at atomistic and coarse-grained levels to investigate the reactivity of lignin, thermal responses of various H-bonding networks of cellulose and its degradation by enzymatic cocktails. We will discuss our recent results from these structural studies that provide useful clues on rational strategies for the efficient degradation.

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