A Multiscale Approach to the Simulation of Lignocellusic Biomass

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Project Goals:
Multiscale methods in theoretical chemistry and molecular simulation are applied to obtain an understanding of the structure, dynamics, and degradation pathways of cellulosic biomass. Using methods that range from accurate quantum chemical calculations to all-atom and coarse-grained molecular dynamics simulation, this project aims to use theory and simulation as a guide for overcoming the recalcitrance to hydrolysis in the production of fuel from biomass.

Cellulosic ethanol production is a two-stage process that involves the hydrolysis of cellulose to form simple sugars and the fermentation of these sugars to ethanol. Hydrolysis of cellulose is the rate-limiting step, and there is a great need to characterize the process with theoretical chemistry and molecular simulations to better understand the complex mechanisms that are involved. The ultimate goal is to generate accurate coarse-grained molecular models that are capable of predicting the structure of lignocellulose before and after pretreatment so that subsequent *ab initio* calculations can be performed to probe the degradation pathways.

Current computational studies include: 1) determining the energy barrier to rotation of free hydroxyl groups in cellulose Iα, 2) characterizing the interfragment and interchain interaction energies in cellulose Iβ with fragment molecular orbital (FMO) calculations of, 3) developing coarse-grained models for crystalline and amorphous cellulose fibers from all-atom molecular dynamics simulations using classical force fields and the effective fragment potential (EFP).

This research is supported under FWP AL-08-330-039 by the Genomic Science Research Program, Office of Biological and Environmental Research and the Scientific Discovery through Advanced Computing program in the U.S. Department of Energy Office of Science.