NREL Highlights

SCIENCE

Supercomputer Provides Molecular Insight into Cellulose

For the first time, scientists calculate the work that enzymes must do to deconstruct cellulose, a fundamental step in converting biomass to biofuel.

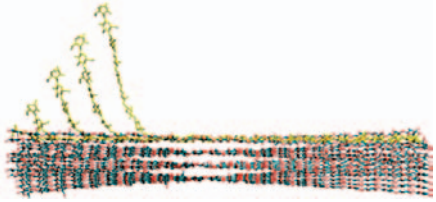
Groundbreaking research at the National Renewable Energy Laboratory (NREL) has used supercomputing simulations to calculate the work that enzymes must do to deconstruct cellulose, which is a fundamental step in biomass conversion technologies for biofuels production. NREL used the new high-performance supercomputer Red Mesa to conduct several million central processing unit (CPU) hours of simulation.

This achievement is important because cellulose is the most abundant biological material on earth, a vast, renewable resource that could help meet the world's energy needs. In plants, cellulose packs into large, crystalline bundles of chains that are incredibly tough to unravel and access. Understanding how to deconstruct these bundles is of vital technological importance.

NREL researchers determined the work needed to decrystallize a single cellodextrin chain in four forms of cellulose called polymorphs. Native plant celluloses (polymorphs Iβ and Iα) exhibit about equal decrystallization work, whereas celluloses polymorph II and especially cellulose polymorph IIII—which are representative of cellulose polymorphs resulting from biomass pretreatment—are substantially easier to decrystallize. This implies that celluloses II and IIII will be less recalcitrant to deconstruction by enzymes compared to natural plant cellulose.

These results will guide the development of enhanced biological catalysts and genetically engineered plants for lignocellulosic biofuels production. The NREL study also provides molecular-level insight into the combined hydrophobic and hydrogen-bonding interactions that form the structural basis of cellulose, which is the primary building block of plants.

Reference: Beckham, Gregg T.; Matthews, James F.; Peters, Baron; Bomble, Yannick J.; Himmel, Michael E.; Crowley, Michael F. "Molecular-Level Origins of Biomass Recalcitrance." Unpublished work. 2010.



Yellow chain shows stages of pulling a cellodextrin chain of cellulose out of a crystalline cellulose microfibril. NREL scientists calculated the thermodynamic penalty that an enzyme must overcome to degrade cellulose for the first time.

Key Research Results

Achievement

NREL scientists used high-performance computational simulations to calculate the work needed to pull a cellodextrin chain out of crystalline cellulose forms.

Key Result

Native plant celluloses showed that significantly greater work is needed to remove the chain from the crystalline region compared to synthetic cellulose.

Potential Impact

These calculations help scientists better understand the biomass recalcitrance problem at the molecular level and will guide rational development of biological catalysts, pretreatment processes, and potentially genetically engineered plants for biofuels production.

NREL
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NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

NREL/FS-2700-50847 • February 2011

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