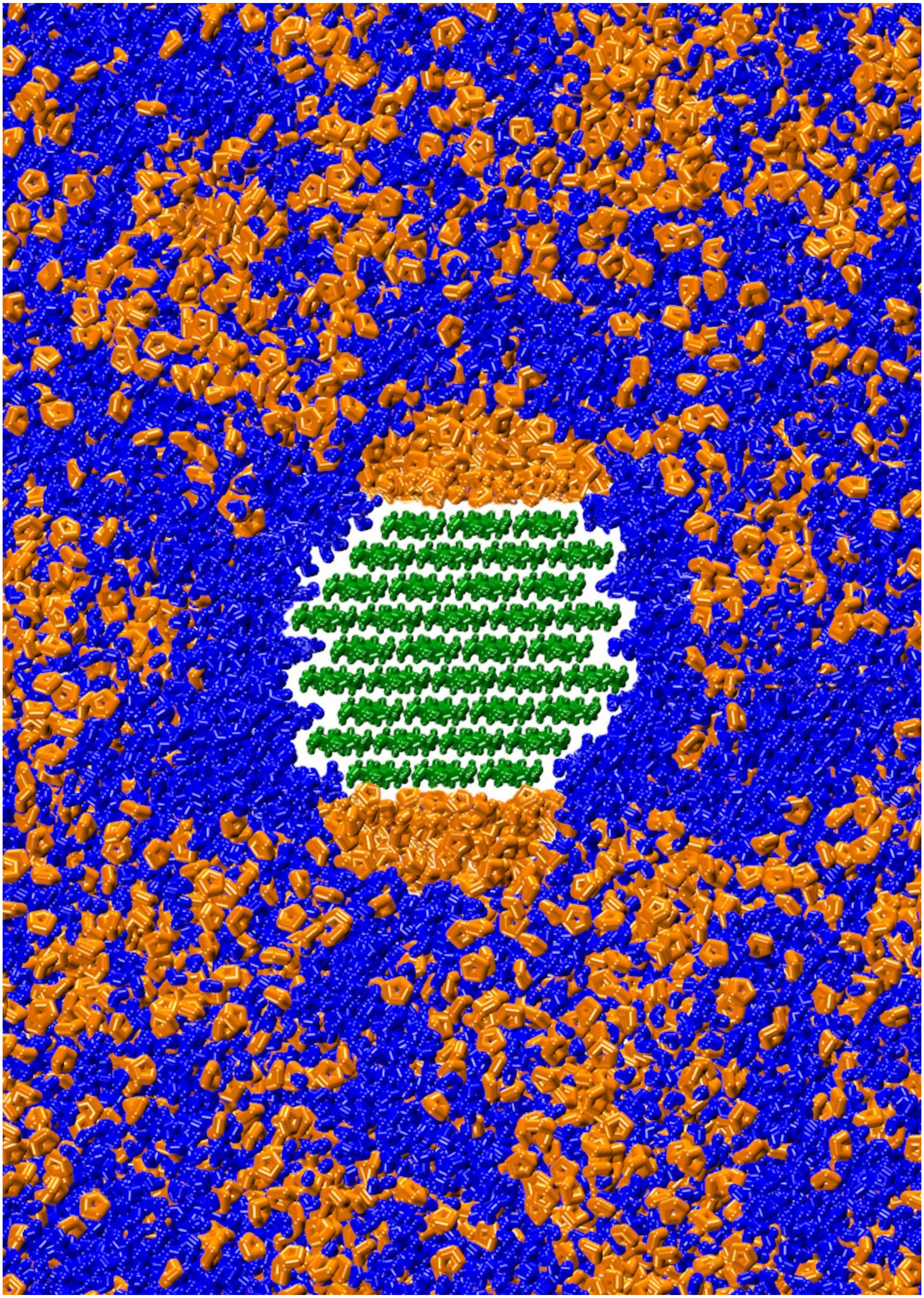
Unraveling the science behind biomass breakdown

October 18 2016



An illustration that demonstrates how THF (orange) and water (blue) phase separate on the surface of cellulose (green), thus facilitating its breakdown. Credit: Barmak Mostofian

Lignocellulosic biomass—plant matter such as cornstalks, straw, and woody plants—is a sustainable source for production of bio-based fuels and chemicals. However, the deconstruction of biomass is one of the most complex processes in bioenergy technologies. Although researchers at the US Department of Energy's (DOE's) Oak Ridge National Laboratory (ORNL) had already uncovered information about how woody plants and waste biomass can be converted into biofuel more easily, they have now discovered the chemical details behind that process.

A team led by Jeremy Smith, a University of Tennessee (UT)-ORNL Governor's Chair and the director of the UT-ORNL Center for Molecular Biophysics (CMB), uses computer simulations to investigate the chemistry of biomass deconstruction. Smith's collaborators from the BioEnergy Science Center, a DOE Bioenergy Research Center led by ORNL, previously developed a pretreatment method for breaking down biomass that initiates delignification, the removal of the rigid plant molecule lignin. The cosolvent enhanced lignocellulose fractionation pretreatment involves aqueous solutions of tetrahydrofuran (THF), a versatile organic solvent. This cosolvent mixture uniquely interacts with cellulose, the main structural component of plant cell walls, to enable its breakdown.

The breakdown of cellulose is essential for its conversion into ethanol, a renewable biofuel made from plants. When scientists understand more details about the process of breaking down cellulose, they will be able to improve the current pretreatment method or find new solvents more efficiently.

In a project led by Barmak Mostofian, a CMB postdoctoral researcher, Jeremy Smith's team created models of up to 330,000 atoms and ran simulations on ORNL's flagship supercomputer—the Cray XK7 Titan located at the Oak Ridge Leadership Computing Facility (OLCF), a DOE Office of Science User Facility—earlier this year. They found that the THF-water cosolvent phase separates on the faces of the crystalline cellulose fiber. These faces are distinct regions with which certain enzymes or molecules can interact. During the phase separation, THF preferentially binds to the hydrophobic, or "water-fearing," faces of cellulose, and water preferentially binds to the hydrophilic, or "water-loving," faces. THF enhances the binding of water molecules to the bonds that link two sugar molecules, which can potentially increase hydrolysis, the chemical breakdown of cellulose by water.

"We saw this phase separation, and we knew it might mean there was chemistry that was taking place on the surface that we hadn't observed, that we hadn't considered before," Micholas Smith, another CMB postdoctoral researcher, said.

The team also found that when they broke the cellulose apart, single chains of cellulose became surrounded primarily by water, while THF—because of its molecular structure—remained bound to the hydrophobic surfaces of cellulose. These results provided researchers with a fine-grained understanding of the chemical properties behind the deconstruction of lignocellulosic biomass.

Researchers say this discovery will help them identify new cosolvents in the future. "This information will help us find the minimum number of things we need to calculate to tell if a solvent is good for lignocellulose," Micholas Smith said. "Hopefully, we will eventually be able to write a program that creates a better screening process for solvents and automatically selects the best ones."

The finding represents a first step toward determining the full pathway the THF-water cosolvent takes to break down cellulose. "Now we are limited to looking at the two end states of the cellulose deconstruction process," said CMB researcher Xiaolin Cheng. "If we can map out the full pathway, that will be more relevant. In the future, with more computing power, we will be able to simulate the degradation pathway of the lignocellulosic biomass to understand what happens between the two endpoints."

More information: Barmak Mostofian et al., "Local Phase Separation of Co-solvents Enhances Pretreatment of Biomass for Bioenergy Applications." *Journal of the American Chemical Society* 138, no. 34 (2016): 10869–10878.

Provided by Oak Ridge National Laboratory

Citation: Unraveling the science behind biomass breakdown (2016, October 18) retrieved 25 April 2024 from https://phys.org/news/2016-10-unraveling-science-biomass-breakdown.html

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