

## **Solvent-induced Membrane Disruption Revealed by Neutron Scattering and Molecular Simulation**

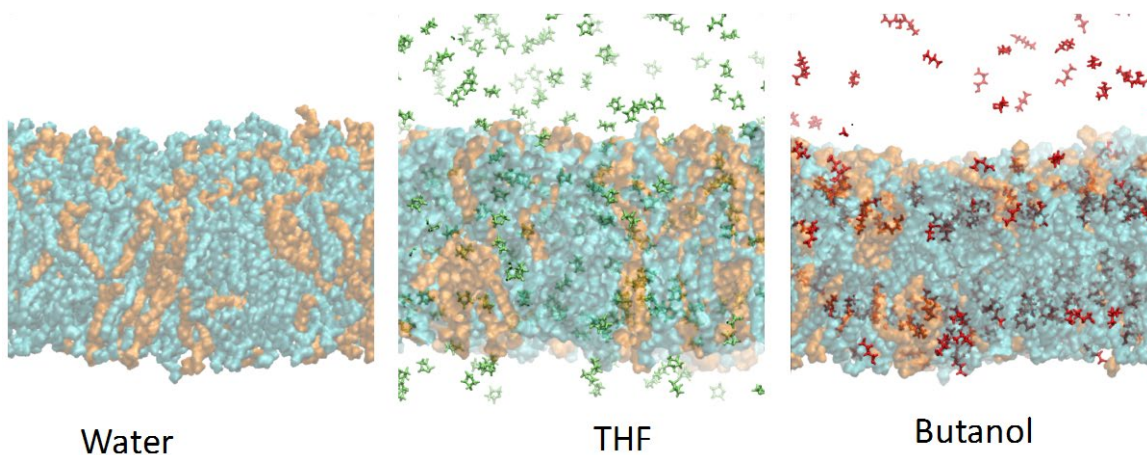
Micholas Dean Smith,<sup>1,2</sup> Sai Venkatesh Pingali,<sup>1</sup> James G. Elkins,<sup>1</sup> John Katsaras,<sup>1</sup> Loukas Petridis,<sup>1</sup> Hugh O'Neill,<sup>1,2</sup> Robert Frank Standaert,<sup>3</sup> Dmitry Bolmatov,<sup>1</sup> Frederick Heberle,<sup>4</sup> Jeremy Smith,<sup>1,2</sup> and **Brian H. Davison<sup>1,2\*</sup> ([davisonbh@ornl.gov](mailto:davisonbh@ornl.gov))**

<sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>University of Tennessee Knoxville, Knoxville, TN, <sup>3</sup>East Tennessee State University, Johnson City, TN, <sup>4</sup>University of Texas Health Science Center at Houston, Houston, TX

<http://cmb.ornl.gov/index.php/research/bioenergy/dynamic-visualization-of-lignocellulose>

**Project Goals: To realize the potential of lignocellulosic biomass to play a major role in generation of renewable biofuels, key limitations in biomass pretreatment and microbial fermentation need to be addressed. For both processing steps, presence of nonaqueous co-solvents can disrupt key biological structures. In the case of biomass, this disruption is desirable, as it facilitates the solubilization and fractionation of lignocellulosic polymers for subsequent cellulosic conversion and lignin valorization. In contrast, the solvents can inhibit fermentation by disruption of microbial cell membranes. The Scientific Focus Area in Biofuels is developing “Visualization of Solvent Disruption of Biomass and Biomembrane Structures in the Production of Advanced Biofuels and Bioproducts” for multiple-length scale, real-time imaging during processing with non-aqueous co-solvents to provide the fundamental information that is needed to improve conversion of renewable lignocellulosic biomass to biofuels.**

A challenge to the efficient conversion of plant biomass to biofuels is obtaining high titers of biofuels and biofuel precursors from microbial fermentation. Key to overcoming this challenge is developing robust fermentative microbes with membranes that can sustain the solvent stressors introduced during the fermentation of pretreated biomass. Here, using a combination of atomistic Molecular Dynamics (MD) simulations and Small-Angle Scattering Neutron Scattering (SANS), we determine how tetrahydrofuran (THF), a residual pretreatment solvent, and butanol, a fermentation product, disrupt a model bacterial membrane composed of 70:30 POPE (1-palmitoyl-2-oleoyl phosphatidylethanolamine) and POPG (1-palmitoyl-2-oleoyl phosphatidylglycerol). Both SANS and MD show that both solvents decrease the thickness of the model membranes, and that the disruption caused by butanol is greater than that by THF. Further, the simulations show that organic solvents increase membrane “fluidity” and that butanol is localized mainly at the lipid head groups, whereas THF is found both around the head groups and the tails. The fundamental understanding obtained here of how nonaqueous solvents can be detrimental to fermentative microbes by disrupting cell membranes will provide a rational basis to develop optimized industrial biomass conversions by limiting inhibition of microbial fermentation.



*Figure: MD snapshots. POPE is cyan, POPG orange, THF green and butanol red. Water molecules not shown.*

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