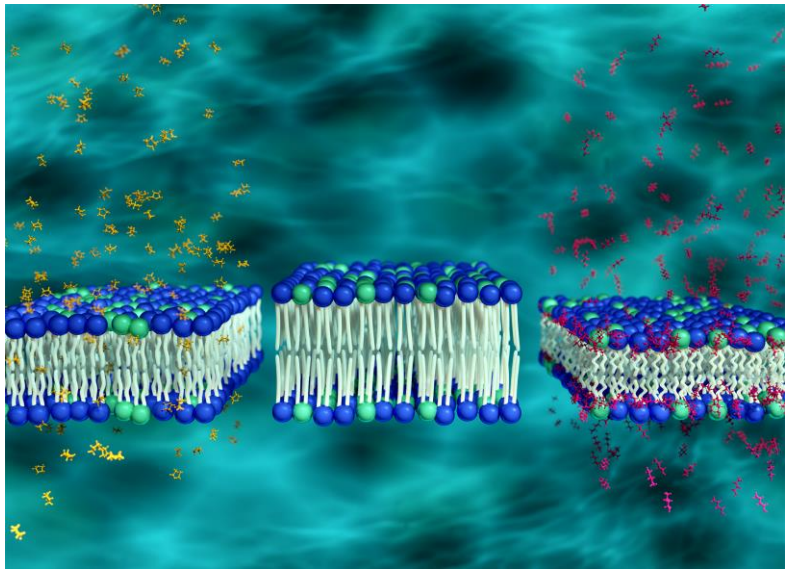
Mechanisms of solvent disruption of bacterial membranes in biofuel production revealed by neutrons and simulations

Objective:

- The presence of organic co-solvents can disrupt microbial membranes, thus inhibiting fermentation and limiting final product titers in biofuel and bioproduct production. The molecular mechanism of this disruption is not well understood or measured.

Approach:

- Using a combination of atomistic Molecular Dynamics (MD) simulations and Small-Angle 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).



Bacterial membrane thinning and disruption by solvents: THF (left), no solvent (center), butanol (right).

Results:

- Both SANS and MD show that both solvents decrease the thickness and increase the fluidity of the model membranes, and that the disruption caused by butanol is greater than that by THF.
- Further, the simulations show that butanol is localized mainly at the interface between the lipid head groups and lipid tails, whereas THF is found predominantly near the lipid tails.

Significance:

- 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.
- Engineering of robust membranes could be based on designing lipid head groups that reduce the accumulation of organic solvents at the head-tail interface.

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