Abstract Submitted
for the SES13 Meeting of
The American Physical Society

Simulation Analysis of the Effects of Partial Charge Modifications on the Hydrophobicity of Lignin CHRISTOPHER CARMONA, Univ of California-Los Angeles and Oak Ridge National Laboratory, Oak Ridge, Tennessee, JEREMY C. SMITH, PAUL LANGN, LOUKAS PETRIDIS, Oak Ridge National Laboratory, Oak Ridge, Tennessee — Lignins are hydrophobic, branched polymers that provide protection against chemical and biological degradation as well as regulate water conduction in plant cell walls. By associating with hemicellulose, lignins form a barrier against effective hydrolysis of plant biomass for cellulosic ethanol production. The effects that the hydrophobicity of lignin has on its association with hemicellulose are not currently well understood. Here, modifications are implemented on three models of lignin based on hydroxycinnamyl aldehydes which are precursors to monolignols along their biosynthetic pathways. Hydroxycinnamyl aldehydes can be genetically engineered into lignin polymers and vary in composition of hydrophobic and hydrophilic functional groups. Each model of lignin is equilibrated beside hemicellulose and then simulated together in an ionized aqueous solution at room temperature. These simulations of partial charge modified lignin, resulting from additional functional groups, provides insight into the overall role that the hydrophobicity of lignin has on its interactions with hemicellulose. Moreover, these insights reveal the effects that inclusion of hydroxycinnamyl aldehydes into the lignin polymer may have on the efficiency of biomass pretreatment for cellulosic ethanol production.

Christopher Carmona
Univ of California-Los Angeles

Date submitted: 04 Oct 2013 Electronic form version 1.4