

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**Structure and diffusion of furans and other cellulose-derived compounds in solvents via MD simulation** BROOKS RABIDEAU, AHMED ISMAIL, RWTH Aachen University, Aachen, Germany — There is now a large push towards the development of energy sources that are both environmentally friendly and sustainable; with the conversion of cellulose derived from biomass into biofuels being one promising route. In this conversion, a variety of intermediary compounds have been identified, which appear critical to successful expansion of the process to an industrial scale. Here we examine the structure and diffusion of these furans and acids derived from cellulose within ionic liquids via molecular dynamic simulation. Ionic liquids have shown the ability to dissolve cellulose with certain ‘green’ benefits over existing, conventional solvents. Specifically, we study the solvation properties of these chemicals by examining the pair correlation functions of solute with solvent, and by exploring the agglomeration and separation of these chemicals from the solvent as well as the hydrogen bonding between species. Additionally, we determine the diffusion constant of these compounds in ionic liquid and aqueous solvents.

Brooks Rabideau  
RWTH Aachen University, Aachen, Germany

Date submitted: 19 Nov 2010

Electronic form version 1.4