Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Wetting Properties of Chemically Modified Surfaces: The role of hydrogen bonding[1] SELEMON BEKELE, MESFIN TSIGE, The University of Akron, Department of Polymer Science, Akron, Ohio — Many industrial processing operations involve the spreading of a liquid on a solid material. Controlling the wetting of one material by another is of crucial importance in such applications as adhesion, coating and oil recovery. A strategy often employed to control the wettability of solid surfaces is a combination of surface patterning and chemical surface modification. In order to understand the effect of surface chemistry on the wetting process, we have carried out all-atom molecular dynamics (MD) simulations of a water droplet spreading on pure and oxidized polystyrene surfaces. Our previous results[2] show that the contact angle generally decreases with increasing oxygen concentration and there is a correlation between the spreading and hydrogen bonding. In this talk, we will present results on the structure and dynamics of the hydrogen bonds in the interfacial region between water and the polystyrene substrate. We will discuss our findings on hydrogen bond lifetimes, time correlations functions and number of hydrogen bonds per water molecule for the hydrogen bonds around the water/polystyrene interface which are found to play a role in the spreading process.

[1]This work was supported by NSF Grant DMR0847580.
[2]*Langmuir* **2013** 29, 13230-13238

Selemon Bekele
The University of Akron, Department of Polymer Science, Akron, Ohio

Date submitted: 13 Nov 2014 Electronic form version 1.4