Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Hydrogen-bond Dynamics at The Interface Between Water and Oxidized Atactic Polystyrene[1] SELEMON BEKELE, Department of Polymer Science, The University of Akron, MESFIN TSIGE[2], Department of Polymer Science, The University of Akron — Hydrogen bonding is very critical to a wide range of systems, from the existence of liquid water at room temperature to the structure of DNA (double helix) and many other biomolecules. The presence of an interface is expected to significantly change the structure and dynamics of the hydrogen bonded network as compared to the situation in the bulk. Understanding the strength and dynamics of hydrogen bonds at surfaces and interfaces has thus stimulated a large and growing body of experimental and theoretical work in recent years. Using all-atom molecular dynamics simulations we have studied the dynamics of hydrogen-bond (H-bond) between water and oxidized atactic polystyrene (aPS). The number of hydrogen bonds between water molecules and oxidized polystyrene is found to monotonically increase with oxygen concentration on the aPs surface. The life-time of this H-bond and the frequency of its formation have also been investigated as a function of oxygen concentration and the results will be presented.

[1]This work is supported by NSF grant DMR0847580.
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Date submitted: 15 Nov 2013 Electronic form version 1.4