Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Structural and dynamic heterogeneity of interfacial water on chemically modified polymer surfaces[1] SELEMON BEKELE, MESFIN TSIGE, The University of Akron, Department of Polymer Science, Akron, Ohio — Using molecular dynamics (MD) simulations, we investigate the structural and dynamical properties of water molecules in a slab of water in contact with atactic polystyrene surfaces of varying polarity. We find that the dynamics of water molecules in the interfacial region slows down with increasing polarity of the polystyrene surface. In addition, the interfacial water molecules exhibit structural and dynamic heterogeneity with respect to diffusion, hydrogen bond distribution and relaxation of the hydrogen bond network. The results obtained enhance our understanding of water structure and dynamics at the polymer/water interface with important implications for such desired functional properties as lubrication, adhesion and friction. Interfacial properties of water at hydrophobic and hydrophilic SAM (Self Assembled Monolayers) surfaces will also be presented for comparison.

[1]This work was supported by NSF Grant DMR1410290

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

Date submitted: 11 Nov 2016 Electronic form version 1.4