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The Behavior of Water at the Interface with Polystyrene[1] SELEMON BEKELE, Tennesse Tech University, MESFIN TSIGE, The University of Akron — Solid-aqueous interfaces are of great importance in many industrial applications ranging from oil recovery to biotechnology. The behavior of interfacial water differs drastically from that of the bulk liquid and strongly depends on the atomistic details of the surface itself. Molecular dynamics simulations have been used extensively to study the structure and dynamics of the interface between a polymeric thin film and water. Using a fully atomistic molecular dynamics simulation, we have examined the structure and dynamics of water and atactic polystyrene (aPS) chains near the aPS-water interface. In this talk, we present results for the contact angle of water and the interfacial surface tension at the aPS-water interface.

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