A large number of industrial processing operations involve the spreading of a liquid on a solid material. Adhesion, lubrication, coating, oil recovery and printing are some examples of practical applications where controlling the wetting of one material by another is of crucial importance. Many applications require good understanding of the interactions that play a role in the spreading and determine the rate of the wetting process. One way to facilitate or inhibit spreading is by chemically modifying the surface of the material on which the liquid rests, thereby varying the interactions at the interface.

Molecular dynamics (MD) simulation is one of the many computational tools being used in the effort to gain an atomistic-level understanding of the mechanisms responsible for the spreading of a liquid on a solid substrate. In addition to addressing the fundamental problem of wetting at the atomistic level, the goal is to provide some level of guidance to industries and experimentalists in the field to design their experiments in a cost effective manner both in terms of money and time. Towards that end, we will present results from atomistic level MD simulations of the spreading behavior of water droplets of different sizes on several oxidized polystyrene surfaces and the role hydrogen bonding plays in this behavior.