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Structural and dynamical properties of water on chemically modified surfaces: The role of the instantaneous surface[1] SELEMON BEKELE, MESFIN TSIGE, The University of Akron, Department of Polymer Science, Akron, Ohio — Surfaces of polymers such as atactic polystyrene (aPS) represent very good model systems for amorphous material surfaces. Such polymer surfaces are usually modified either chemically or physically for a wide range of applications that include friction, lubrication and adhesion. It is thus quite important to understand the structural and dynamical properties of liquids that come in contact with them to achieve the desired functional properties. 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 density of water molecules and the number distribution of hydrogen bonds as a function of distance relative to an instantaneous surface exhibit a structure indicative of a layering of water molecules near the water/PS interface. For the dynamics, we use time correlation functions of hydrogen bonds and the incoherent structure function for the water molecules. Our results indicate that the polarity of the surface dramatically affects the dynamics of the interfacial water molecules with the dynamics slowing down with increasing polarity.

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