

Abstract Submitted
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Interfacial Structure and Dynamics of the liquid/liquid interface between Polydimethylsiloxane and Polystyrene¹ MESFIN TSIGE, University of Akron — Many important phenomena in biology, chemistry and in various fields involve processes that occur at the interface between two immiscible liquids. A molecular level understanding of such interfaces is crucial for insight into the complex dynamics that are observed at such interfaces. In this study, atomistic molecular dynamics simulations were performed to study the structural and dynamical properties of the liquid/liquid interface between two immiscible polymers, polydimethylsiloxane (PDMS) and polystyrene (PS). A series of simulations is carried out to examine the temperature and molecular weight dependence of the orientation of molecules at and away from the interface, intermolecular correlation at the interface, interfacial tension and interfacial thickness. The results from these detailed simulations will be presented.

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