518f Determination of Interfacial Properties of Polysiloxane-Water Systems Using Molecular Dynamics Simulations

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Polysiloxanes are widely used as adhesives in a wide range of applications. Debonding can occur by water displacing the polysiloxane molecules at the surface. To improve our understanding of this process, we have performed molecular dynamics (MD) simulations of polysiloxanes such as polydimethylsiloxane (PDMS) and polyethylmethylsiloxane (PEMS) in the presence of water, with the long-term goal of studying how water molecules effect debonding at the surface. Knowledge of the basic interfacial properties of a multicomponent system, such as the surface tension, contact angle, and diffusion constant, are essential to obtain the proper dynamic behavior in a molecular simulation of adhesion and wetting processes. Two classical force fields were tested in explicit-atom simulations of 10^5 or more particles to determine which best reproduced the experimentally measured liquid/vapor surface tension and contact angle for water on the surface of PDMS and PEMS. We present results for the dependence of the surface tension on chain length, end-group functionality, and interaction potential cutoff.