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Interfacial Properties of Polydimethylsiloxane-Water Systems[1]
AHMED E. ISMAIL, GARY S. GREST, MARK J. STEVENS, Sandia National Labs, MESFIN TSIGE, Southern Illinois University at Carbondale, DAVID R. HEINE, Corning — Polydimethylsiloxane (PDMS) is a main constituent of silicone adhesives, which have a wide use as adhesives. Often these adhesives are used as sealants. The interaction between water and PDMS is of fundamental importance. To improve our understanding at the molecular level, we have performed molecular dynamics (MD) simulations of PDMS 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. Explicit-atom simulations of 10^5 or more atoms were used to determine liquid-vapor surface tension and the contact angle for water on the surface of PDMS. We present results for the dependence of the surface tension on chain length and end-group functionality.

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