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Molecular Dynamics Simulations of Poly(dimethylsiloxane) - Silica Interfaces JAMES SMITH, OLEG BORODIN, GRANT SMITH, University of Utah — Molecular Dynamics simulations using new quantum chemistry based interactions between Poly(dimethylsiloxane) (PDMS) and silica surfaces were conducted to explore the chain behavior near the interface between 300 and 500 K. The effects of surface chemistry particularly the presence of hydroxyl and trimethyl-silyl groups at the interface were examined. The PDMS chain dynamics, as measured by the mean squared displacement of backbone atoms, were strongly affected by the surface chemistry and intermolecular interactions. The PDMS structure near the interface depended upon the type of surface group on the silica surface and its concentration. The significance of intermolecular forces such as hydrogen bonding, electrostatics etc. will be discussed.

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