

Abstract Submitted  
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**Dynamics of water on self-assembled monolayers**<sup>1</sup> J. MATTHEW D. LANE, MICHAEL CHANDROSS, MARK J. STEVENS, GARY S. GREEST, Sandia National Labs, CHRISTIAN D. LORENZ — Nanoscale surface interactions of water at polymeric interfaces are important for a number of applications including biophysics, nanofluidics and MEMS devices. Using molecular dynamics simulations we investigate the fundamental properties of water at interfaces for a variety of water models and surfaces. We report results for the contact angle and wetting dynamics of TIP3P and SPC/E water on self-assembled monolayers (SAMs) of alkylsilanes on amorphous silica and alkanethiols on gold with various hydrophilic and hydrophobic head groups. For comparison we also investigate water interactions on bare amorphous silica substrates. Simulations of the dynamics of water confined between two surfaces coated with SAMs will also be presented.

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