

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Diffusion of Water through Methyl- and Hydroxyl-Terminated Poly(Dimethylsiloxane)¹ AHMED E. ISMAIL, GARY S. GREY, DAVID R. HEINE², MARK J. STEVENS, Sandia National Laboratories, MESFIN TSIGE, Southern Illinois University — Both experimental and numerical reports of the diffusion constant of water through poly(dimethylsiloxane) (PDMS) show variances of nearly an order of magnitude. We use molecular dynamics simulations to calculate the diffusion constant for both methyl- and hydroxyl-terminated PDMS chains. We examine the effects of both concentration and chain length. For a single water molecule, we find that diffusion depends strongly on the initial location of the molecule, as the “caging” phenomenon reported by Mller-Plathe can occur. At intermediate concentrations, we observe the formation of dimer and trimer water clusters, leading to lower diffusion rates; at concentrations above the reported aggregation limit of 0.1 wt %, we observe the onset of phase segregation.

¹Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract No. DE-AC04-94AL85000.

²Present address: Corning

Ahmed E. Ismail
Sandia National Laboratories

Date submitted: 07 Dec 2008

Electronic form version 1.4