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Structure and dynamics of water near the interface with oligo(ethylene oxide) self-assembled monolayers AHMED E. ISMAIL, GARY S. GREST, MARK J. STEVENS, Sandia National Laboratories — Oligo(ethylene oxide) self-assembled monolayers (OEO SAM's) deposited on Au are the prototypical materials used to study protein resistance. Recently, protein resistance has been shown to vary as a function of surface coverage and to be maximal at about two-thirds coverage, not complete coverage. We use molecular dynamics simulations to study the nature of the interface between water and the OEO SAM for a range of SAM coverages. As SAM coverage decreases, the amount of water within the OEO monolayer increases monotonically; however, the penetration depth of the water shows a maximum near the experimentally-found maximal coverage. As the water content increases, the SAM-water mixture becomes harder to distinguish from bulk water. Since the oxygen atoms of OEO are hydrogen bond acceptors, a hydrogen bond network forms within the SAM-water mixture. The water molecules diffuse freely within the monolayer and exchange with the bulk water. Because the monolayer becomes increasingly like bulk water as the coverage decreases, proteins stay in their bulk soluble conformation and do not adsorb. Sandia 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.

Ahmed Ismail
Sandia National Laboratories

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