

Abstract Submitted  
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**Polyethylene oxide hydration in grafted layers.**<sup>1</sup> ELENA DORMIDONTOVA, ZILU WANG, Physics Department and Institute of Materials Science, University of Connecticut, Storrs, CT — Hydration of water soluble polymers is one of the key-factors defining their conformation and properties, similar to biopolymers. Polyethylene oxide (PEO) is one of the most important biomedical-applications polymers and is known for its reverse temperature solubility due to hydrogen bonding with water. As in many practical applications PEO chains are grafted to surfaces, e.g. of nanoparticles or planar surfaces, it is important to understand PEO hydration in such grafted layers. Using atomistic molecular dynamic simulations we investigate the details of molecular conformation and hydration of PEO end-grafted to gold surfaces. We analyze polymer and water density distribution as a function of distance from the surface for different grafting densities. Based on a detailed analysis of hydrogen bonding between polymer and water in grafted PEO layers, we will discuss the extent of PEO hydration and its implication for polymer conformation, mobility and layer properties.

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