

Abstract Submitted
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Conformation and hydration of surface grafted and free polyethylene oxide chains in solutions.¹ UDAYA DAHAL, Department Dept. of Physics and Institute of Materials Science, Univ. of Connecticut, ZILU WANG, Dept. of Physics and Institute of Materials Science, Univ. of Connecticut, ELENA DORMIDONTOVA, DDept. of Physics and Institute of Materials Science, Univ. of Connecticut — Due to the wide application of polyethylene oxide (PEO), ranging from biomedicine to fuel cells, it is one of the most studied polymers in the scientific world. In order to elucidate detailed molecular-level insights on the impact of surface grafting on PEO conformation, we performed atomistic molecular dynamics simulations of PEO chains in solution and grafted to a flat gold surface in different solvents. We examined the hydration as well as conformation of the free chain compared to the grafted polymer in pure water and mixed solvents. We find that grafted chains are stiffer and have a stronger tendency to form helical structures in isobutyric acid or mixture of isobutyric acid and water solution than the free chains in corresponding solutions. For grafted chains exposed to pure water the random coil conformation is retained at low grafting density, but becomes stretched and more dehydrated as the grafting density or temperature increases.

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