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Structure of End-Grafted Polymer Brushes – A Molecular Dynamics Study IAN ELLIOTT, TONYA L. KUHL, ROLAND FALLER, UC Davis — Molecular dynamics simulations of a polar polymer brush in a polar solvent are presented using a coarse-grained approach. Chain extension is heavily influenced by temperature as expected. Chains extend far from the surface at high temperature, while surface adsorption at a weakly attractive surface dominates at low temperature. Increasing grafting density leads to greater chain extension due to excluded volume effects under all conditions, consistent with previous scaling analysis. Polymer depletion regions are found near the surface even at very high grafting densities indicating a chain orientation normal to the surface close to the grafting points. Radial distribution functions reveal that the grafting pattern does not affect the overall brush configuration beyond the first five monomers of each chain as long as the surface is homogeneously covered.

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