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**Polymer Loop Formation on a Functionalized Hard Surface: Quantitative Insight by Comparison of Experimental and Monte Carlo Simulation Results**

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The grafting of telechelic polystyrene terminated with carboxylic acid end groups from the melt onto an epoxidized silicon wafer is examined experimentally to monitor the kinetics of the grafting and loop formation processes. These ellipsometry and fluorimetry results are quantitatively correlated with bond fluctuation Monte Carlo (BFMC) simulations, which provides unique insight into the process of polymer loop formation. Specifically, this correlation provides a calibration of the fluorescence intensity to the amount of singly bound chains present on the surface, revealing that about 80% of the bound chains form loops on the surface at the longest reaction time studied, and provides the time evolution of singly and doubly bound chains during the reaction. Moreover, this correlation is broadly applicable and can be used to readily monitor the impact of a broad range of reaction conditions (e.g., temperature, telechelic concentration, surface density of functional groups) on the loop formation process. This correlation, therefore, provides a method to access fundamental information that is not available by experiment alone, and yet is required to tailor surface properties through adjusting the coverage and fraction of loops in the grafted layer and to correlate surface sensitive properties to specific grafted layer structure.