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Brush formation at the reactive surface from end-functionalized polymer YE ZHANG, FANG YIN, DMITRY BEDROV, GRANT SMITH, Materials Science & Engineering, University of Utah — Brush formation at the reactive surface from end-functionalized polymer Ye Zhang, Fang Yin, Dmitry Bedrov, Grant D. Smith Department of Materials Science and Engineering, University of Utah, Salt Lake City, Utah, 84112 We use bond-fluctuation Monte Carlo simulation to explore the polymer brush formation by absorbing end-functionalized polymer chains onto reactive surface in melt and good solvent. By examining the dynamically determined brush structure, we find that: (1) penetration of the chains from bulk to the brush significantly reduces upon formation of the brush; (2) brushes become more extended: perpendicular to surface upon formation of the brush; (3) heterogeneous doubly-bonded loops (chains with both end-groups reacted with surface): later formed loop has larger brush height and shorter lateral end spacing than earlier formed ones; (4) adding non-reactive chains into the melt promotes the percentage of doubly-bonded loops in the brush. We also compare the dynamically determined brush structure with equilibrium brush structure by allowing end- groups to move on the surface. Furthermore, we compared the brush structure with singly-bonded brush with half chain length.

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