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Controlling co-monomer distributions in bulk and surface tethered random copolymers LAWRENCE STRICKLAND, JAN GENZER, CAROL HALL, North Carolina State University — Tuning the chemical composition and co-monomer sequence distribution in random copolymers (RCPs) affects profoundly their physico-chemical characteristics. We present the results of discontinuous molecular dynamics (DMD) simulations of “coloring” reactions performed by reacting B species with A-type homopolymers to create A-*co*-B copolymers both in bulk and tethered on an impenetrable, flat surface and discuss the effects of varying system temperature, chain length and surface density on copolymer blockiness. In bulk systems, decreasing the system temperature (i.e., reducing parent homopolymer solubility) results in RCP with a more random-blocky co-monomer character. Coloring of short homopolymers tethered to flat surfaces leads to copolymers whose blockiness is similar to those RCPs formed in the bulk. Increasing the chain length and/or increasing the surface density – thereby increasing chain-chain interactions and restricting access to monomers near the surface – results in RCPs with blocky (in some cases nearly diblock) monomer distributions. We also explore the means by which long blocky copolymers are formed as a function of the system temperature (relative to theta-temperature).

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