Polymer Brushes as "Smart" Surfaces

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"Smart" surfaces can change their structure and composition in response to subtle changes in the surrounding environment. Using continuum self-consistent field calculations in real space, we have studied the structure and stimuli-response of three smart polymer brushes: (1) Thermo-response of grafted poly(N-isopropyl acrylamide) (PNIPAM) in water. Here we use a concentration-dependent Flory-Huggins parameter obtained from experiments, and have studied the structure and thermo-response of PNIPAM brushes as a function of chain length and grafting density. (2) Solvent-response of uncharged diblock copolymer (DBC) brushes. Here we have studied the effects of copolymer chain length, copolymer composition (length ratio of the two blocks), grafting density, and A-B incompatibility on the brush height and surface switchability of DBC brushes. (3) Stimuli-response of charged two-component polymer brushes. Here we have further studied DBC brushes with one block charged. When charge effects dominate, it is ineffective to switch the brush surface by different solvents. Rather, the ionic strength, solution pH and applied electric field are more effective, with sharp transitions for the surface-switching. For these complex systems, however, it is critical to understand the interplay between different stimuli in order to better design smart surfaces for targeted applications.