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**Towards Improving the Targeting Efficiency of End-Functionalized Polymer Brushes** CHUN-CHUNG CHEN, ELENA E. DORMIDONTOVA, Department of Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, Ohio 44106
— Functionalized protective polymer layers are actively used in drug/gene delivery. By means of computer simulations, we study the interactions between a polymer layer end-functionalized by ligands and a surface containing receptors. We analyze the influence of ligand valence and the polymer layer architecture on binding efficiency of the ligands. Multivalent ligands are shown to substantially improve the efficiency of targeting through cooperative binding but the distance between the functional groups relative to the spacing of receptor sites is crucial to the success of the targeting. Thus, multivalent ligands with a branch length shorter than the receptor spacing turned out to be less efficient than monovalent ligands. We also studied bidisperse polymer brushes consisting of short non-functional and long functionalized polymers. We found that bidisperse structure of the polymer layer considerably improves accessibility of the functional groups leading to the stronger attraction between the polymer layer and receptor surface. The bidisperse structure of a polymer brush can be combined with multivalent ligands in order to greatly improve the binding of a functionalized polymer brush with receptor surfaces.

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