Role of PMMA in Amphiphilic Polymer Brush for Optimal Increase of Absorbance in Dimer
Gold Nanoparticle

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We studied the self-assembled amphiphilic gold nanoparticles (Au-NP) by the dissipative particle dynamics (DPD). The polymer brushes, which are grafted on Au core, consists of hydrophilic poly(ethylene glycol) (PEG) and hydrophobic poly(methyl methacrylate) (PMMA). For Au-NP, constituent beads, which are building blocks of DPD representing groups of atoms, molecules, and fractions of polymers, have been systematically modeled in coarse-graining manner. The most efficient Au-NP dimer model for sensing has been found in terms of the size of Au core, the thickness of the polymers, and the distance of Au cores in dimer. It was found that Au core became the largest when the amounts of amphiphilic polymers were roughly same and in the range of dimerization condition that we found, dimer distance was closest when PMMA is less compared to PEG. This study unveil that the unseen distributions of polymers and Au cores, which are hard to distinguish in experiment, affect to the dimerization for the sensing capability.