Self-assembly of mono and dimer gold nanoparticles grafted with amphiphilic polymers via dissipative particle dynamics

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By modeling amphiphilic gold nanoparticles by grafting hydrophilic (PEG) and hydrophobic (PMMA) polymers, we found specific conditions to make single and dimer nanoparticles in polar (water) and polar aprotic (DMF) solvents. From simulations, single nanoparticle is well formed in DMF, where PEG is stretched out to the solvent, than in water, where many gold precipitates are still found. In particular, when the ratio of the number of beads of PEG and PMMA is same in water, the gold nanoparticle becomes the largest (i.e. ~6.3 nm diameter of Au). Also, the ternary phase diagram of gold, PEG, and PMMA in a fixed amount of water has been constructed to find out the formation condition of dimer. For a stable dimer, the distance of two nanoparticles has been found to be ~15.5 nm. To do this study, dissipative particle dynamics (DPD) has been used. The method utilizes the concept of coarse-graining constituent molecule of target material, which realized by the building block of DPD, bead.