Polymer-Grafted Nanoparticle and its Application in Drug Delivery

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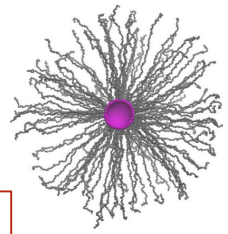
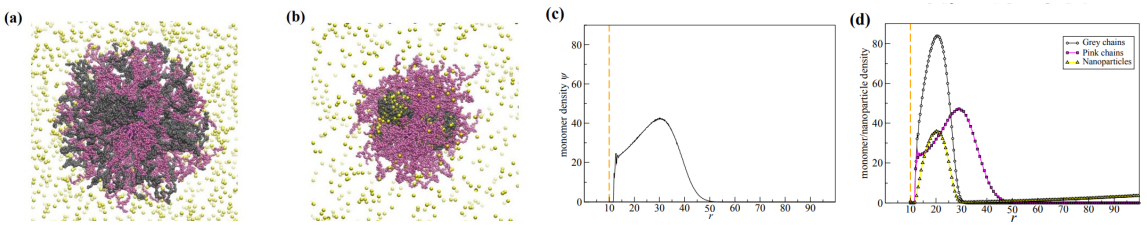


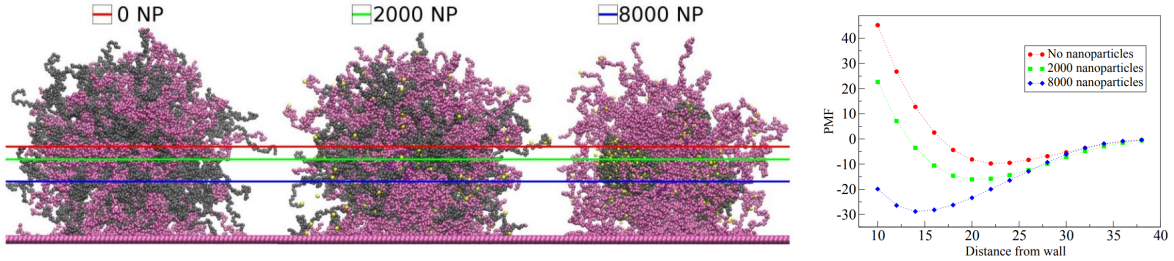
Introduction

This study explores a novel mechanism for controlling the surface properties of polymer coated colloids using targeted ("sticky") nanoparticles which attract monomers of certain polymer species. In our study, colloids are coated by two types of tethered polymer chains having different chemical properties. Attraction of nanoparticles to the monomers of one polymer type causes these polymer chains to contract towards the grafting surface, rendering the other type more exposed to the environment. Thus, the effective surface properties of the colloid are dominated by the intended polymer type. We use Coarse Grained Molecular Dynamics (CGMD) simulation to demonstrate that introducing nanoparticles which interact preferentially with certain types of polymers makes it possible to switch between different surface properties of the colloid. This mechanism can in principle be exploited in drug delivery systems and self-assembly applications.

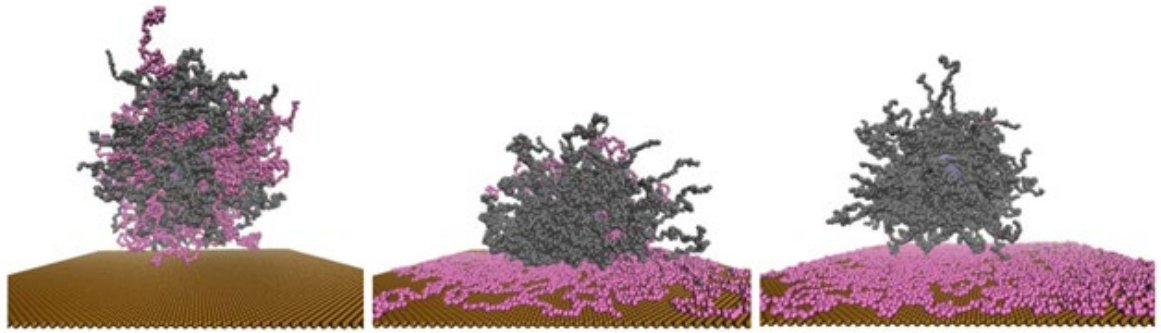


Nanoparticles (yellow) interacting with grey polymer chains contract these chains, which effectively increases the exposure of pink chains. (a) The hairy chain-coated colloid ball before infiltration of nanoparticles into it. (b) The hairy ball after contracting the grey polymer chains via sticky nanoparticles. (c) Average monomer density profile of the polymer chains (grey and pink taken together) as a function of the radial distance from the colloid before introducing the nanoparticles to the system (d) Monomer density profile of the pink and grey polymer chains (separately resolved), and the nanoparticle density as a function of the radial distance from the colloid after introducing 8000 nanoparticles into the system.

Results



The equilibrium distance between colloid and wall decreases as the number of sticky nanoparticles in the system increases. Horizontal lines show the location of the center of the colloid sphere for systems with 0, 2000 and 8000 sticky nanoparticles. (Nanoparticles not shown.) PMF of the colloid center of mass coordinate as a function of distance from the wall for these three systems.



for some applications, it might be useful to consider the situation where the strength of the bond between the polymer chains and colloid is comparable to the other interaction energies in the system. In this case the chain-colloid bonds are dynamic (breakable). The following figure shows snapshots from the time evolution of a system comprised of 100 pink chains and 100 grey chains. Each grey chain is grafted to a random position on the colloid surface via a static bond, while each pink chain is grafted to the colloid surface via a dynamic bond.

Ozmaian, Masoumeh, Brayden A. Freitas, and Rob D. Coalson. "Controlling the Surface Properties of Binary Polymer Brush-Coated Colloids via Targeted Nanoparticles." *The Journal of Physical Chemistry B* 123.1 (2018).