



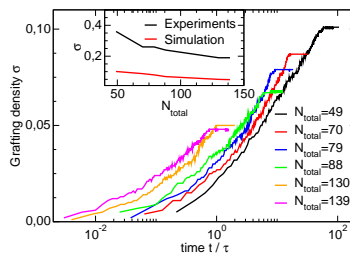
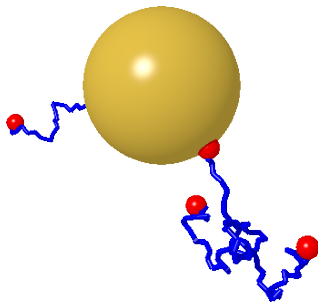
Obtaining High Grafting Density Shells

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Project

Recently we found that the normal diffusion and adsorption of star polymers in simulation could not generate the desired experimental polymer shells with high grafting density on the gold nanoparticle's surface (see Figure). As more molecules are adsorbed on the surface, the new star polymers are difficult to approach the particle's surface. This kinetic barrier inhibits the preparation of high grafting polymer shells in simulation.

Now the question is: how to overcome this high kinetic barrier to obtain the experimental grafting density polymer shells? The goal of this bachelor project is to explore the possible simulation procedures, such as changing temperature or chemical potential, to answer these questions.



Required Skills and Main Work:

- Familiar with C language, gnuplot. Interested in programming.
- Modifying and running the code.
- Discussion and comparison to experimental results.

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