Investigating the pH Dependent Surface Structure of Citrate Coated Silver Nanoparticles

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One of the most common coatings for silver nanoparticles is citrate because of its low cost and relatively benign biological effects. The citrate molecules do not bind very strongly to the nanoparticle surface; instead their surface binding is mainly favorable because the citrate molecules replace bound water molecules which then have more configurational freedom. Experiments have observed that citrate coated nanoparticles change in their surface charge as the pH of the solution changes, which is often attributed to the protonation or deprotonation of citrate molecules on the surface. However, there is little simulation evidence of this hypothesis. In our work, we build computational models of citrate coated silver nanoparticles under the assumption that the mixture of citrate protonation states present in solution are what would be expected from the pKa's of citrate. We then calculate the surface charge of the resulting nanoparticles and find a correlation to experimental zeta potential measurements. We also generally quantify the surface coating structure of the nanoparticles.