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Effects of functional groups and ionization on the structure of alkanethiol coated gold nanoparticles DAN S. BOLINTINEANU, J. MATTHEW D. LANE, GARY S. GREST, Sandia National Laboratories — We report fully atomistic molecular dynamics simulations of alkanethiol coated gold nanoparticles solvated in water and decane. The structure of the coatings is analyzed as a function of various functional end groups, including amine and carboxyl groups in different neutralization states. We study the effects of charge in the end groups for two different chain lengths (10 and 18 carbons) and different counterions (mono- and divalent). For the longer alkanes we find significant local phase segregation of chains on the nanoparticle surface, which results in highly asymmetric coating structures. In general, the charged end groups attenuate this effect by enhancing the water solubility of the nanoparticles. Based on the coating structures and density profiles, we can qualitatively infer the overall solubility of the nanoparticles. The asymmetry in the alkanethiol coatings is also likely to have a significant effect on aggregation behavior. More importantly, our simulations suggest the ability to modulate end group charge states (e.g. by changing the pH of the solution) in order to control coating structure, and therefore control solubility and aggregation behavior.

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