

Abstract Submitted
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Functionalized Au nanoparticles in solution GARY S. GREY, J. MATTHEW D. LANE, Sandia National Labs — The properties of functionalized Au nanoparticles in decane and water were studied by large-scale explicit atom, molecular dynamics simulations. Gold nanoparticles functionalized with S-(CH₂)₉-X alkanethiols chains (X = COOH or CH₃) were studied at the liquid-vapor interface and in the bulk. The structure of the functional groups on the nanoparticle was found to depend strongly on the end group and solvent. At the interface methyl terminated nanoparticles repel the water and move toward the vapor while in decane, the decane molecules engulf the nanoparticle. In the bulk, results for the nanoparticle/nanoparticle pair correlation function and nanoparticle diffusion will be presented as a function of nanoparticle concentration. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

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