

Abstract Submitted  
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**Mechano-Chemical Stability of Gold Nanoparticles Coated with Alkanethiolate SAMs**<sup>1</sup> BRIAN HENZ, U.S. Army Research Laboratory, TAKUMI HAWA, MICHAEL ZACHARIAH, University of Maryland and National Institute of Standards and Technology — Molecular dynamics simulations are used to probe the structure and stability of alkanethiolate self-assembled monolayers (SAMs) on gold nanoparticles. We have observed that the surface of gold nanoparticles become highly corrugated by the adsorption of the SAMs. Furthermore, as the temperature is increased, the SAMs dissolve into the gold nanoparticle, creating a liquid mixture at temperatures much lower than the melting temperature of the gold nanoparticle. By analyzing the mechanical and chemical properties of gold nanoparticles at temperatures below the melting point of gold, with different SAM chain lengths and surface coverage properties, we have determined that the system is metastable. The model and computational results that provide support for this hypothesis are presented.

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