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Structural Properties and Phase Transitions in Small Gold Nanoclusters YANTING WANG, SERGEY RASHKEEV, Idaho National Laboratory — Small gold nanoclusters (below 5 nm in diameter) exhibit good catalytic activity. Molecular dynamics simulations combined with the parallel tempering method have been used to investigate the bulk and surface structural properties and phase behavior of small gold nanoclusters (10^1-10^4 atoms). For small clusters, the transition from solid to liquid does not occur at a definite temperature. Instead, one gets a temperature range in which the transition state from solid to liquid is observed, and this range become broader for nanoclusters with smaller number of atoms. In this work, we perform an analysis of structural and dynamic properties of gold nanoparticles of different sizes and show that the nature of the solid-liquid phase transition in very small nanoparticles (with tens of atoms) is radically different from that of the mid-sized ones (10^2-10^4 atoms). The surface characteristics of the particle (the presence of low-coordinated atoms at the surface and the dynamic fluxionality, i.e., an ability of the surface to reconstruct) that define its catalytic behavior are also investigated and analyzed.

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