

Abstract Submitted
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Is the Debye-temperature a useful concept at the nanometer scale? Insights from *ab initio* free energy calculations of Au₁₃ and Au₁₂Fe nanoclusters GHAZAL S. SHAFAI, MARISOL ALCANTARA ORTIGOZA, TALAT S. RAHMAN, University of Central Florida — We have calculated the phonon density of states, specific heat, and mean-square vibrational amplitudes of the five lowest-lying isomers of Au₁₃ and two of Au₁₂Fe nanoparticles, as dictated by their Helmholtz free energy. We find the vibrational entropic contributions to not affect the energy ordering of the isomers. We show that the highest phonon frequencies shift to slightly higher energies in the hybrid clusters: a signature of alloying. As expected the density of vibrational states differs significantly from the Debye model for bulk systems. The definition of the “Debye temperature” for the nanocrystal thus becomes ambiguous and depends very much on how it is calculated. In particular it neither correlates uniquely with atomic bond strengths nor does it relate to the maximum phonon frequency. The discrete phonon spectrum of nanoparticles is thus needed to describe the *exact* mean square displacement or the temperature dependency of the heat capacity. Work supported by DOE Grant DE-FG02-07ER46354

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