Abstract Submitted
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Ab Initio **Calculations for the Surface Energy of Silver Nanoclusters**[1] BHARAT MEDASANI, IGOR VASILIEV, Department of Physics, New Mexico State University, Las Cruces, New Mexico 88003, YOUNG HO PARK, Department of Mechanical Engineering, New Mexico State University, Las Cruces, New Mexico 88003 — We apply first principles computational methods to study the surface energy and the surface stress of silver nanoparticles. The structures, energies and lattice contractions of spherical Ag nanoclusters are calculated in the framework of density functional theory combined with the generalized gradient approximation. Our calculations predict the surface energies of Ag nanoclusters to be in the range of $1-2$ J/m^2. These values are close to the bulk surface energy of silver, but are significantly lower than the recently reported value of 7.2 J/m^2 derived from the Kelvin equation for free Ag nanoparticles[2]. From the lattice contraction and the nearest neighbor interatomic distance, we estimate the surface stress of the silver nanoclusters to be in the the range of $1-1.45$ N/m. This result suggests that a liquid droplet model can be employed to evaluate the surface energy and the surface stress of Ag nanoparticles.

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[2]K. K. Nanda *et al.*, Phys. Rev. Lett. **91**, 106102 (2003)

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