

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Optical properties of medium size noble and transition metal nanoparticles JUAN C. IDROBO, Vanderbilt University, SOKRATES T. PANTELIDES, Vanderbilt University and Oak Ridge National Laboratory — Using first-principles methods within time dependent density functional theory and the local density approximation (TDLDA) the absorption spectra of medium size (~ 20 -80 atoms) silver, gold and copper nanoparticles have been calculated. The nanoparticles are fcc fragments with different aspect ratios. We find that in the case of Ag nanoparticles is well reproduced by classical electrodynamics theory based in Mie's formalism, using the dielectric function of bulk Ag and taking into account the nanoparticle shape. For the case of Cu and Au, there is a similarity in the overall features of the quantum mechanical and classical spectra, but no detailed agreement. We will discuss the role that the d-electrons among all the different elements and the surface states play in controlling the optical properties of the nanoparticles. This work was supported by GOALI NSF grant (DMR-0513048), DOE, the Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, and Alcoa Inc.

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Date submitted: 28 Nov 2008

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