

# Optical Properties of Noble Metal Clusters: Comparing Non-local Classical and TDDFT Calculations

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The Localized Surface-Plasmon Resonance (LSPR) in quantum-sized noble metal clusters (~1-3nm) is being widely used in numerous applications in biological sensing/detecting technology. The LSPR depends on size, composition and geometry of the clusters. It is well known that the resonance energy of the LSPR is strongly red-shifted with increasing aspect ratio of the clusters as is well described by classical local theory [1-3]. In model clusters of Au and Ag, full quantum calculations using time-dependent density-functional theory (TDDFT) have shown deviations from this classical behavior [4]. The different contributions to the spectra have also been analyzed [5,6]. To study the deviations in the behavior of the LSPR in particles having very small sizes (~1nm), the non-local nature of the bulk dielectric response has been incorporated into classical electrodynamics through a density-dependent hydrodynamic model [7]. Moreover, good agreement with experiments is found by using these non-local effects described in the local analogue model (LAM) [8].

In this work we present a comparative study of the full quantum analysis of model noble-metal nanorods of different sizes and aspect ratios with classical local and non-local calculations. For the non-local classical calculations, where the non-locality is described by the LAM, complex Lorentz-Drude fitted dielectric functions [9] are used. On the other hand, the TDDFT calculations are carried out using the time evolution method by means of the octopus code.

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